OPTIMIZATION: A PERSPECTIVE ON IMPROVING AN ETHYLBENZENE PRODUCTION DESIGN

by
Derrick Cochrane Marchant

A thesis submitted to the faculty of The University of Mississippi in partial fulfillment of the requirements of the Sally McDonnell Barksdale Honors College.

Oxford
May 2015

Approved by

____

Advisor: Dr. Adam Smith

____

Reader: Dr.John O'Haver

____

Reader: Dr. Paul Scovazzo

Acknowledgements

There are many people and factors to thank that have built and pushed me throughout my academic career. My parents, Eddy and Cindy, have pushed me from the start and are always there for encouragement. I would like to thank Dr. Adam Smith for being my thesis advisor and helping me as an undergraduate student in class and for this thesis. I would like to thank Dr. Paul Scovazzo and Dr. John O'Haver in the same manner as well and also for reading my thesis as second and third readers. I thank my fellow classmates Cary Robbins and Jasper Ring for working in a group together and passing Plant Design I together. Cary Robbins provided the base case and optimized case process flow diagrams and stream tables seen throughout. Jasper Ring helped with the PRO/II simulation, the bulk of the sample calculations, and provided the selectivity/conversion graph.

Abstract

The goal of optimization in a chemical process or system involves improving an existing design or a combination of devices. In the case of an established process such as the ethylbenzene production process investigated here, the optimization involves improving an established process and choosing the best available case within a set of constraints that also considers maximizing the economic bottom line. An objective function must be selected for an optimization problem which defines the achievable goal. The objective function of the optimization process presented here is to minimize the estimated annual operating cost (EAOC). An EAOC takes in to account all the necessary variables that add up to the yearly operating costs of a chemical process such as utility and raw material costs. The secondary objective function presented here is maximizingthe net present value (NPV) which is directly related to minimizing the EAOC. The NPV takes in to account the recurring costs of plant operation over a plant's expected lifetime. Both objective functions are assessed and considered. By defining a number of constraints and decision variables related to the objective function, an optimization problem becomes a dynamic and creative exercise. The report included contains an evaluation of defined constraints, decision variables, and proposed changes and an optimized design utilizing the engineering resources available. The optimized design focuses on making a catalyst change to maximize the efficiency of the reactor section and also on changing the raw material feed to directly reduce the raw material cost of operation. Safety of the plant's operation follows a full economic analysis and detailed process description of the optimized design.

List of Figures

List of Tables

List of Abbreviations and Nomenclature

Distillation Column:

m_D: Mass flow rate in the distillate stream

m_{Dl}: Liquid mass flow rate in the distillate stream

m_B: Mass flow rate in the bottoms stream

m_{Bl}: Liquid mass flow rate in the bottoms stream

V_{Dv}: Volumetric flow rate of the vapor in the distillate stream

V_{Bv}: Volumetric flow rate of the vapor in the bottoms stream

V_D: Total volumetric flow rate of the vapor in the distillate stream

V_B: Total volumetric flow rate of the vapor in the bottoms stream

ρ_D: Density of the distillate stream

ρ_B: Density of the bottoms stream

R: Reflux ratio

v_D: Linear velocity of the distillate stream

v_B: Linear velocity of the bottoms stream

D_D: Diameter of column required by distillate stream

D_B: Diameter of column required by bottoms stream

$N_{theoretical}$: Number of theoretical trays required in the distillation column

ε: Efficiency of each tray

H: Height of the distillation column

Vessels:

m: Mass flow rate of the feed into the vessel

V: Volumetric flow rate of the feed into the vessel

ρ: Density of the feed stream

t: Holdup time of the vessel

Vol: Volume of the vessel

k: Height to diameter ratio

H: Height of the vessel

D: Diameter of the vessel

Heat Exchangers:

T_{pf}: Process stream feed temperature

T_{pm}: Process stream intermediate temperature

T_{pe}: Process stream effluent temperature

T_{wf}: Water stream feed temperature

T_{wm}: Water stream intermediate temperature

T_{we}: Water stream effluent temperature

T_{LMl}: Log mean temperature difference of latent heating

T_{LMs}: Log mean temperature difference of sensible heating

U_l: Latent heat transfer coefficient of the water stream

U_s: Sensible heat transfer coefficient of the water stream

m_w: Mass flow rate of the water stream

H_{wf}: Enthalpy of the water at the feed temperature

H_{wm}: Enthalpy of water at the intermediate temperature

H_{we}: Enthalpy of water at the effluent temperature

Q_t: Total duty of the heat exchanger

Q_l: Latent duty of the heat exchanger

Q_s: Sensible duty of the heat exchanger

A_t: Total heat transfer area of the heat exchanger

A_l: Latent heat transfer area of the heat exchanger

A_s: Sensible heat transfer area of the heat exchanger

Reactors:

V_c: Volume of the catalyst in the reactor

L: Length of the catalyst in the reactor

D: Diameter of the reactor

L_R: Length of the reactor

V_R: Volume of the reactor

Pumps:

m: Mass flow rate of feed stream into pump

V: Volumetric flow rate of feed stream into pump

ρ: Density of feed stream into pump

Pf: Pressure of feed stream into pump

P_e: Pressure of effluent stream out of pump

ΔP: Pressure rise in pump

ε: Efficiency of pump

W: Pump work

Table of Contents

Introduction

The production of ethylbenzene is an important process that predominantly plays a role in the co-production of styrene. 99% of ethylbenzene produced is involved in consumption in the production of styrene. Styrene is the main precursor for the production of polystyrene, a common thermoplastic material [1]. The alkylation of benzene and ethylene in the presence of a catalyst is the primary reaction that produces ethylbenzene. However, additional side reactions may occur under certain circumstances whereby higher degrees of benzyl alkylations are formed. The side reactions form undesirable products that must be separated and reacted with excess benzene to form additional ethylbenzene.

The purpose of this report is to design and optimize a new ethylbenzene (EB) plant. A case study with a certain amount of base case plant information is available through the senior design class, Ch E 451, under the instruction of Dr. Adam Smith during the fall 2014 academic term. Analysis and evaluation of the case study is necessary to make improvements and recommendations for an optimized design. The EB plant produces 80,000 tonne/yr of 99.8% ethylbenzene with an impurity of less than 2 parts per million (ppm) of diethylbenzene. Numerous changes are available for the base case EB plant within the case study. These changes affect certain parts of the plant and thus affect the design of the overall plant.Choices and decisions to accept or decline the changes proposed are a part of the optimization process that forms the bulk of this report.

The major changes and improvements considered forthe EB plant include: optimizing the base case, making a catalyst change, making a feed change, or making both a catalyst and feed change. This report analyzes each change and defends the decisions through justifications and guidelines available.

Theory and Background of Optimization

Optimization is the process of improving an existing situation, device, or system such as the chemical process of ethylbenzene production investigated here [2]. In order to set up an optimization problem, an objective function is selected and constraints are placed on a specified number of decision variables. An objective function is simply a mathematical function that one either minimizes or maximizes to obtain an improved process. The objective function for this process is to maximize the net present value (NPV) of the ethylbenzene production or, in other terms, to minimize the estimated operating annual costs (EAOC). The recurring costs of the operation are discounted to obtain a NPV while the capital costs of the full operation are annualized to obtain the EAOC. Both of the objective functions considered are interchangeable in the economic analysis of the process. Decision variables are independent variables considered whereby one has the ability to control and vary based on justifications. Constraints are the limitations of the decision variables and consider the range of operation of certain variables [2]. The constraints for this optimization process are to produce 80,000 tonne/yr of ethylbenzene product, maintain an ethylbenzene product at 99.8% purity, and also maintain an impurity of less than 2 ppm of diethylbenzene in the ethylbenzene product.

For the investigation represented in this report, both a base-case and a topological approach identify considerations for improvement and represent the starting point of optimization. The goal of optimization is to improve a process, therefore, it is necessary to start from an ethylbenzene production process that is already defined. For the senior plant design course, Ch E 451, a case study is provided with a fully operational process for the production of ethylbenzene. The case study contains the base case used for the optimization. This report elaborates in detail the important considerations of the base case before an optimization approach is undertaken.

The production of an ethylbenzene product at 99.8% mole purity with less than 2 ppm diethylbenzene at a rate of 80,000 tonne per year are the primary constraints of this optimization research. Using the given base case as a guideline, a unique optimized design achieves a more efficient and less expensive overall plant design using the resources at hand. Table 1, found below, is the cost summary of the base case and a logical starting point for the optimization.

Table 1 - Base Case Cost Summary (All Fixed Capital Investment (FCI) and Estimated Annual Operating Costs (EAOC) are represented in millions.)

Equipment	FCI	% of FCI
Fired Heater	\$2.333	40
Heat Exchangers	\$1.373	23
Pumps	\$0.224	4
Towers	\$0.535	9
Vessels	\$1.383	24
Total	\$5.848	100

Cost Type	EAOC	% of EAOC
Natural Gas	\$2.556	2.81
HPS	\$1.767	1.94
LPS	\$1.120	1.23
CW	\$0.039	0.04
Electricity	\$0.010	0.01
Benzene	\$68.516	75.37
Ethylene	\$16.894	18.58
Total	\$90.902	100
HPS, credit	-\$2.092	
LPS, credit	-\$1.332	

An initial analysis of Table 1 shows that the Fired Heater makes up the largest portion of the fixed capital cost of the plant operation. The fired heater also uses the utility of natural gas which makes up the third most percentage of the EAOC behind the raw materials of benzene and ethylene. A next step is to investigate the operation of the fired heater, the use of natural gas as a fuel, and also the necessity of the fired heater to the production of ethylbenzene.

Using Table 1 and knowledge of justifications from a process condition matrix (PCM), a topological optimization approach is nextimplemented, eliminating or rearranging equipment according to process condition and heuristic guidelines [2]. Table 3, below in the results and discussion section, contains the PCM for the base case.

The details for the decisions made for the topological approach are found in the results and discussion section.

The objective function of this optimization process is to improve the net present value as much as is feasible; therefore, a full economic analysis of the plant is necessary. A sensitivity analysis aids in the approach to this economic analysis by highlighting components to be considered and evaluated. Below, in Figure 1, are the main components from the base case information considered. An initial sensitivity analysis covering a ±30 percent difference change in each component focuses the approach and direction of the optimization process.

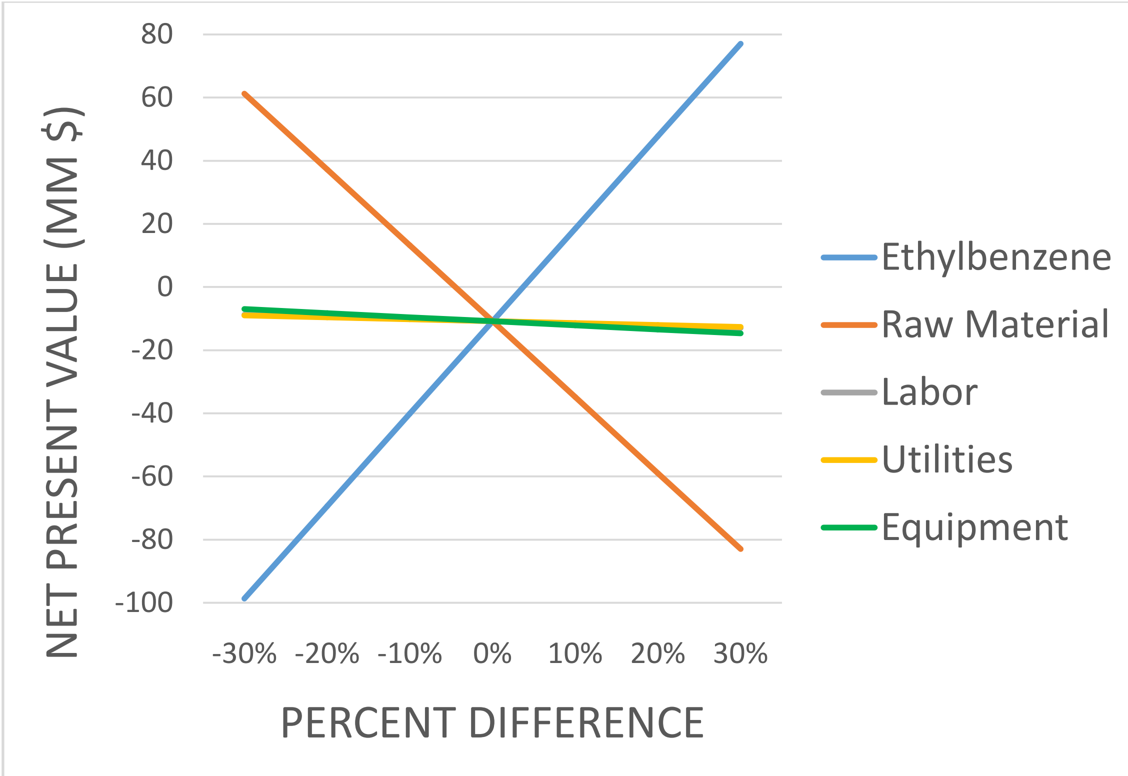


Figure 1 - Sensitivity analysis of the major economic components plotting net present value vs. %Difference

An initial consideration from Figure 1 is that the ethylbenzene production has the greatest positive impact on the NPV of the operation. The raw materials, ethylene and benzene, have the greatest cost and negative impact on the NPV of the operation.

Figure 2, below, contains an enhanced sensitivity analysis featuring the three components that have less of an effect on the net present value as they increase or decrease in value. After a full economic analysis of the base case design, the net present value is approximately -$10.86 million as can be seen in Figure 2 as well.

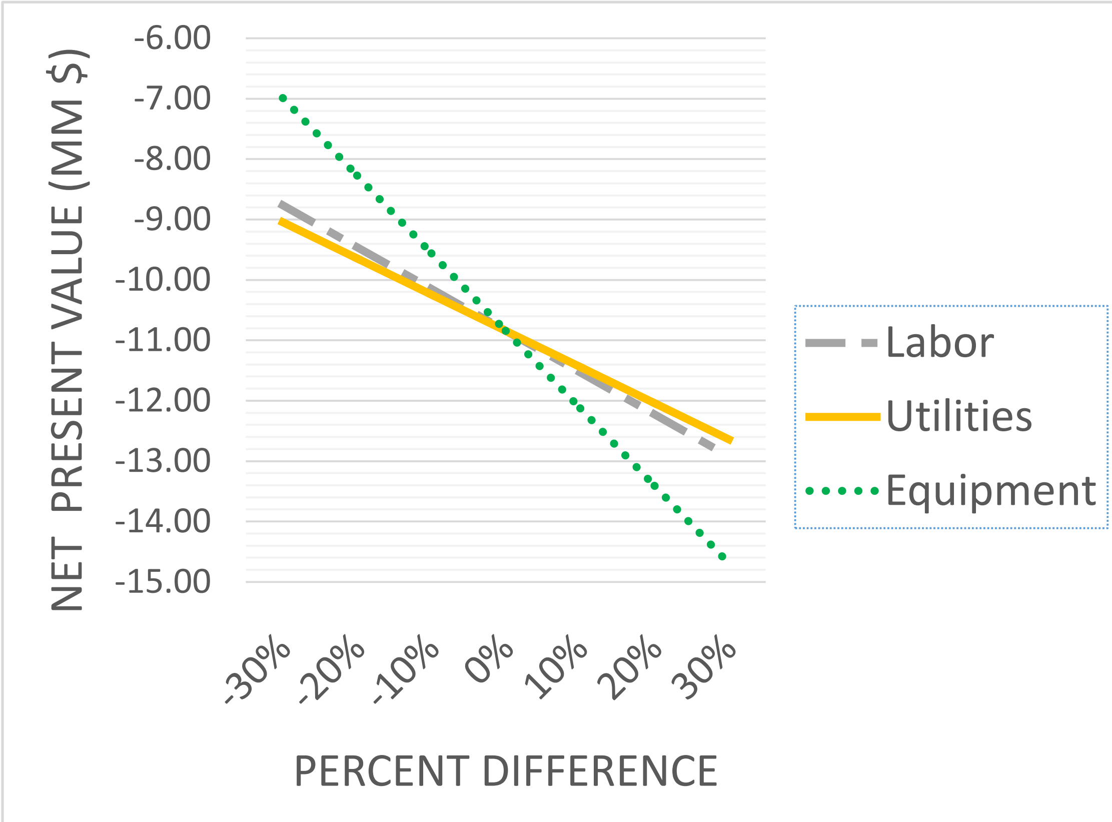


Figure 2 – Enhanced Sensitivity Analysis highlighting Labor, Utilities, and Equipment

Results and Discussion

Analysis of the base case design and process justifications

Given a case study for the production of ethylbenzene, a PRO/II simulation program that obeys the constraints supplied further analyzes the overall ethylbenzene production process. A process flow diagram (Appendix A) for the base case is found in the appendix as well as the respective stream table (Appendix B). A primary objective for the analysis of the base case is to gain a deeper understanding of the major sections of the plant, meet the design specifications, and define the Estimated Annual Operating Cost (EAOC) to consequentlyanalyze the net present value (NPV) of the plant.

An appropriate thermodynamic model for the PRO/II simulation is necessary to provide as accurate as possible data for analysis. The selection of the SRK SIMSCI model is used in both the base case analysis and optimized plant design simulations. This model applies to calculations with aromatic, non-polar hydrocarbons. The production of ethylbenzene predominantly uses these compounds.

Looking through each major section of the plant while analyzing the base case, the process conditions for justification are summarized in a process condition matrix (PCM) that is seen below in Table 3. Conditions of special concern are marked with an X in the diagram. The X identifies which pieces of equipment are closely reviewed for conditions of special concern. [2]

Table 2 – Process condition matrix highlighting conditions of special concern

	Reactors and Separators					Other Equipment				
Equipment	High Temp	Low Temp	High Pres.	Low Pres.	Non-Stoich. Feed	Comp.	Exch.	Htr.	Valve	Mix
R-301	X		X		X					
R-302	X		X		X					
R-303	X		X		X					
R-304	X		X		X					
V-301										
V-302										
V-303										
V-304										
T-301										
T-302										
H-301								X		
E-301							X			
E-302							X			
E-303										
E-304										
E-305										
E-306										
E-307										
E-308										
E-309										
P-301						X				
P-302										
P-303										
P-304						X				
P-305						X				
PCV stream 14									X	

Evaluating the process conditions identified above, improvements are either justified or recommended for the conditions of the particular piece of equipment and overall process topology.

The elevated temperature associated with the reactor train (R-301 – R-303) allows for a favorable reaction conversion when compared to lower conditions below the 400°C limitations. A decision to maintain the elevated temperature of the reactor train is made after analyzing the conversion-selectivity curves of the reactor train seen below in Figures 3 and 4. Data for the streams can be seen in Appendix A.2 as part of the base case stream tables. Also seen below is a visualization of the base case reactor train labeled Figure 5. To accommodate for the increasein temperature, special materials need to be used and are considered further in the report.

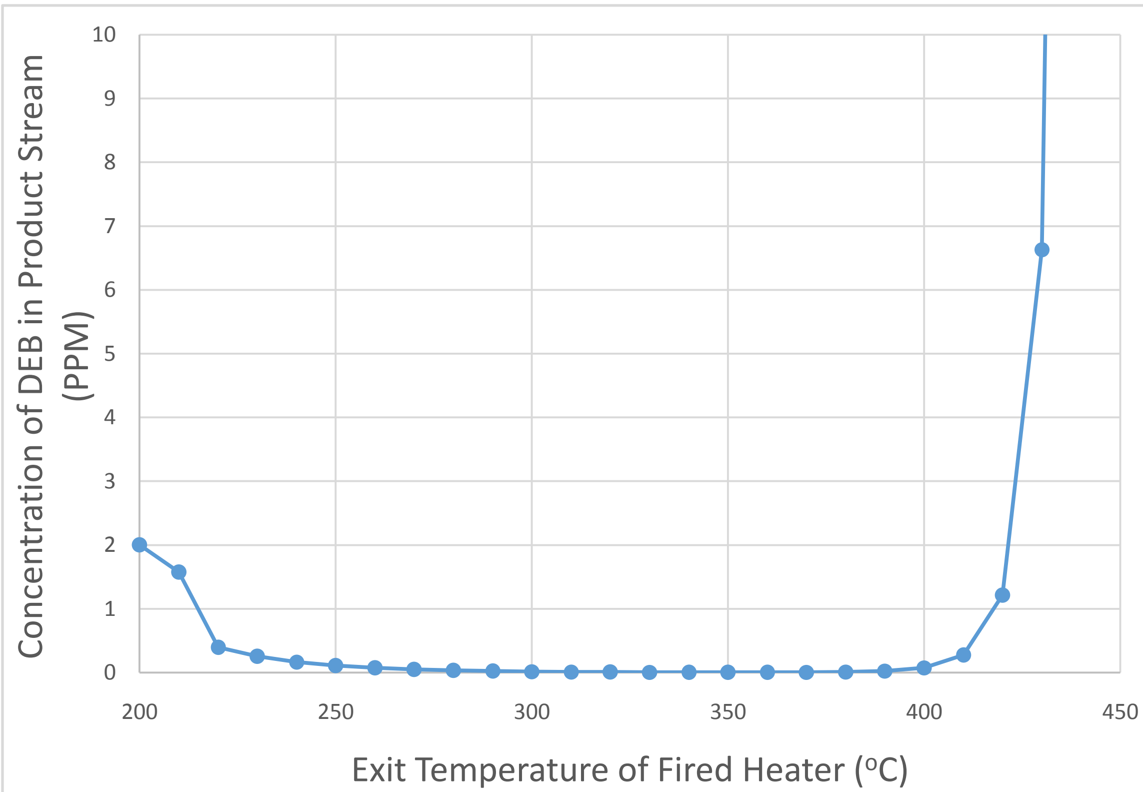


Figure 3 - Concentration of diethylbenzene (DEB) in product stream vs. Exit temperature of theFired Heater (H-301)

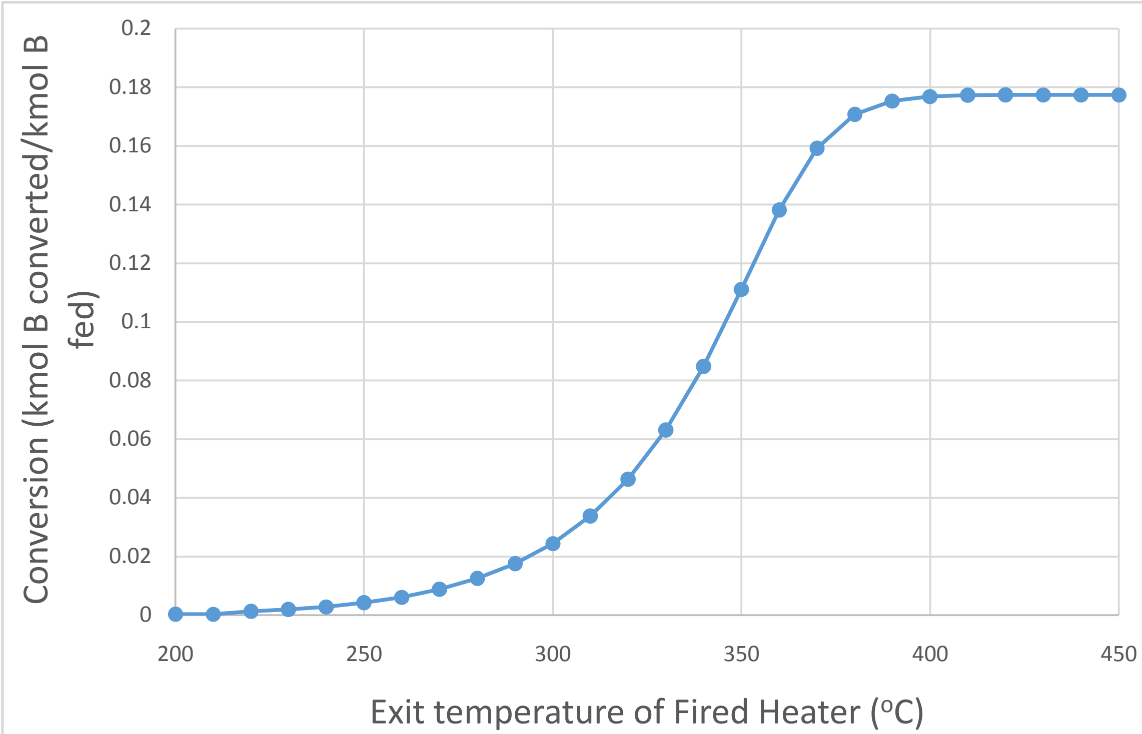


Figure 4- Conversion of benzene to ethylbenzene vs. Exit temperature of the Fired Heater (H-301)

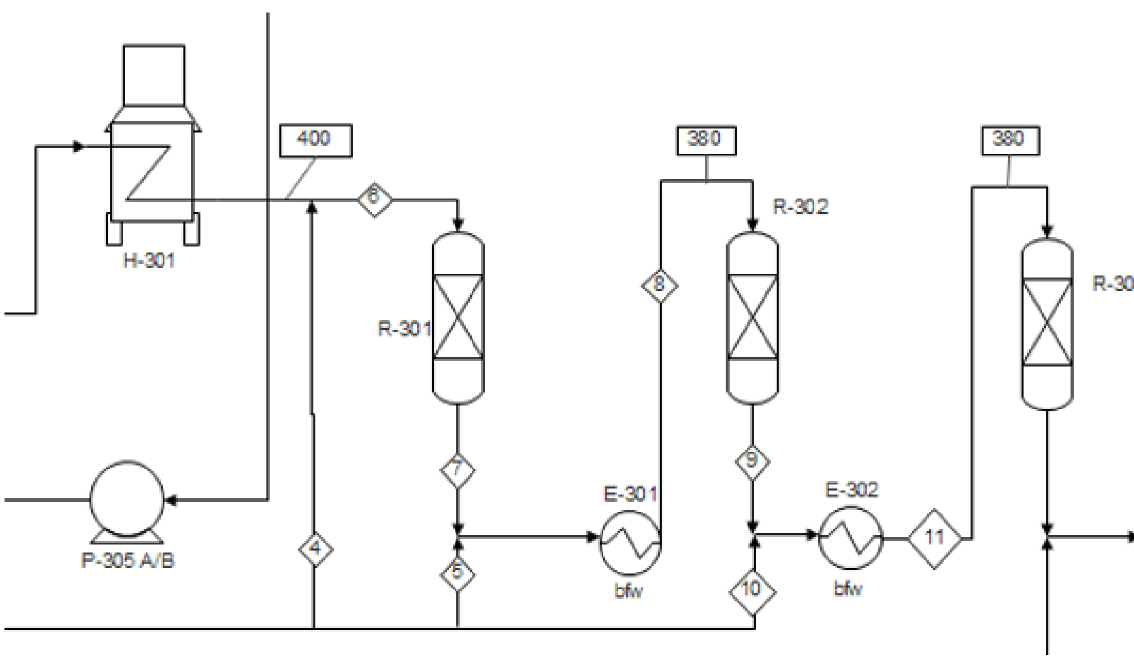


Figure 5 – Base case reactor train

The reactions taking place within the reactor train all have experimental data provided as well as kinetic data in the case study. As a result, the overall reaction is kinetically controlled. No further considerations are evaluated involving changing the reactions other than suppressing one or more of the side reactions based on undesirable products. The summary of reactions is given below.

$$C_6H_6 + C_2H_4 \rightarrow C_6H_5C_2H_5 \qquad (1)$$

Benzene Ethylene Ethylbenzene

$$C_6H_5C_2H_5 + C_2H_4 \rightarrow C_6H_4(C_2H_5)_2 \qquad (2)$$

Ethylbenzene Ethylene Diethylbenzene

$$C_6H_4(C_2H_5)_2 + C_6H_6 \rightarrow 2C_6H_5C_2H_5 \qquad (3)$$

Diethylbenzene Benzene Ethylbenzene

$$C_6H_5CH_3 + 2C_2H_4 \rightarrow C_6H_5C_2H_5 + C_3H_6 \qquad (4)$$

Toluene Ethylene Ethylbenzene Propylene

The inherent reactor design is reviewed and a series vs. parallel setup is considered.R-301 in the reactor train produces the highest ratio of ethylbenzene to diethylbenzene. This results from R-301 having the highest benzene to ethylene ratio in the inlet feed. Since diethylbenzene is an undesirable product and a chemical that must be recycled and reacted further, an initial consideration is to simply suppress the production of it. Diethylbenzene must be accounted for in the second separation section, T-302, and subsequent recycle stream if it is not suppressed. The suppression is accomplished by splitting the initial reactor train feed and feeding it to two separate reactors in parallel. This split in feed eliminates the production of diethylbenzene by way of reaction (2). With the suppression of reaction (2), the separation and recycle of diethylbenzene is unnecessary. The eventual reaction of diethylbenzene in reaction (3) is also an unnecessary consideration and is eliminated.

The non-stoichiometric feed of benzene compared to the ethylene feed ensures a high conversion to ethylbenzene. An 8:1 ratio of benzene to ethylene is employed for the base case. The minimum ratio of benzene to ethylene is found in the reactor train at the inlet feed to R-303. The ratio is 4.36:1 of benzene to ethylene feed and this ratio is utilized for the optimization of the plant design.

Large outlet pressures at P-301, P-304, and P-305 arenecessary in order to run the reactors at high pressures. Enforced materials are required to withstand the elevated pressures. Multiple pumps for different process conditions and topological arrangements are considered.

The Fired Heater, H-301, needs to produce an effluent at a higher temperature than that of high pressure steam (254°C). [2] This is necessary for proper reactor conditions but requires special heating to reach temperatures in excess of 400°C. Also, lowering the reactor feed stream temperature is evaluated based on the reactor design.

The pressure control valve (PCV) on stream 14 has a large pressure drop warranting the possible use of a turbine to recapture some of the energy lost to the pressure drop. Because stream 14 passing through the valve is predominantly all liquid, little useful work is recovered from the stream and the use of a turbine is not a recommended addition to thetopological optimization process.

The fuel gas product in Stream 15 is burned instead of being recycled or stored. This burning approach is the easiest and cheapest way to deal with the left over ethane and propylene and is not considered any further than the base case evaluation. Similar amounts in the overhead fuel gas from the flash vaporization process is utilized in the optimized design. An appreciable amount of benzene raw material feed can occur if the temperature of the separator is too high. A lower temperature of this two-phase separator is reviewed and optimized to minimize the loss of raw materials.

Summary of proposed changes and improvements

The major objective of the optimization process is improving the topological design as well as improving the use of sensitive components, such as raw material feeds, in order to maximize the profit of the plant. The profit margin of a plant is the difference between the value of the products and the cost of the raw materials. Table 3 below showcases that the profit margin for the base case is small initially, therefore, many improvements are necessary to make the economic potential a more positive number. Also below, in Figure 6, the process concept diagram highlights the main inputs and outputs of the plant. A process concept determines the chemical components that enter with the inputs feeds and exit as product outputs. All of the reactions, both desired and undesired, that take place in the process limit the performance of equipment such as the reactors involved.

Table 3 – Profit margin for the production of ethylbenzene

Economic Potential	
$27,468,394.38	per year
$3,301	per hour
$0.34	per kg

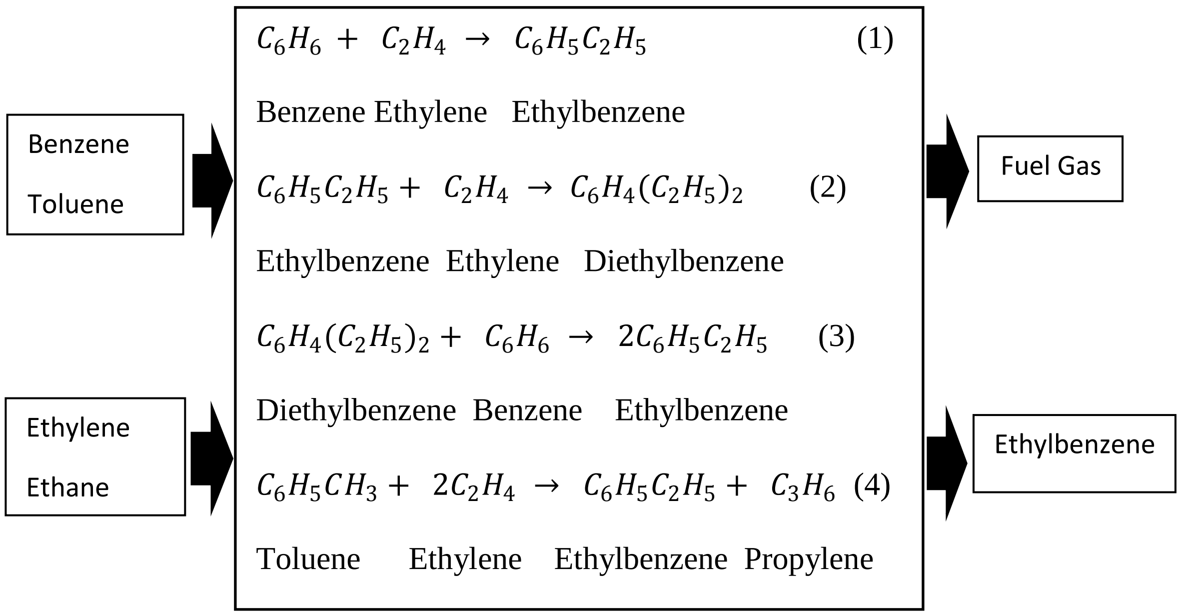


Figure 6 – Process concept diagram highlighting feed components and effluent components

A number of changes and a summary of the major improvements is included below. Each changed is evaluated and implemented based on the contribution to the objection function of improving the economic impact of the plant.

The first major change considered is to implement a new catalyst. The new catalyst costs \$8/kg and expects to have a lifetime of only 4 years. The project length is 12 years after start up so the catalyst needs to be changed at least 3 times over this span. The catalyst provides enhanced suppression of diethybenzene production and can operate at a maximum of 500 °C. The operation of our reactor train is optimal between 400 °C and 500 °C in our design, so the catalyst meets these requirements. After running the newer catalyst in PRO/II simulations, the feed rates are reduced allowing more controllability over the raw materials cost. As seen earlier in the sensitivity analysis, the raw materials cost hugely impacts the economic growth of the process. The new catalyst therefore greatly affects the net present value of the plant positively.

The second change consists of purchasing and implementing a lower grade of benzene feed. The new feed contains 10% toluene and 90% benzene and costs \$0.85/kg. The implementation of the lower grade of feed is possible given the constraints by adjusting the raw material feed rates in the PRO/II simulations. This change is also economically attractive, reducing the raw material component cost drastically. The design of the reactor scheme allows for the suppression of diethylbenzene production and increases the controllability of the feed rates even further. The choice of implementing the lower grade of benzene will have a positive impact on the optimization design set forth in describing thus far.

The third proposed change involves implementing both the new catalyst and lower grade of benzene. This option is the chosen change for the optimized plant design and has the best economic impact based on this process design. By changing to the lower grade of benzene a direct reduction in the raw material feed cost is observed. A more efficient reaction scheme with a controllable suppression of diethylbenzene occurs with the utilization of the new catalyst as well.

The fourth proposed change calls for optimizing the base case with no catalyst change or purchase of lower grade of benzene feed. This is a viable option, however, the added benefits of reduction of feed costs and controllability of the reaction scheme as it relates to the economic analysis are too good to not implement. Therefore, simply optimizing the base case is not the best change proposed in the design.

After a detailed analysis of the individual proposed changes given, the third proposed change is chosen to best optimize the plant's design. After consideration of the process conditions of concern in the base case the topological approach is now implemented. An optimized plant design continues by removing certain equipment and adjusting accordingly.

The removal of the bottom recycle stream as a result of implementing the new catalyst and using a parallel reactor design leads to the first major topological improvement. The suppression of diethylbenzene is the most important contribution to the removal of the second separation and recycle loop. The removal of equipment contained within this recycle is as follows: T-302, E-308, E-309, V-304, P-303 A/B, P-304 A/B, the bottom of H-301, R-304. A direct reduction in the fixed capital investment of equipment results from the elimination of this bottom recycle stream. A major reduction in the relatively high annual utility cost of natural gas in the bottom part of H-301 also results with this elimination. A more concentrated focus on the simple separation of ethylbenzene from the reactor effluent without regards to the diethylbenzene continues next.

The second major topological improvement considered involves deciding between a series versus parallel design to the reactor. In a series design, the benzene to ethylene ratio of the feed to each subsequent reactor reduces with the last reactor having the lowest ratio. In the base case this ratio is 4.36:1 benzene to ethylene. In a parallel reactor design, the benzene to ethylene ratio is kept constant and controlled to meet the minimum feed ratio of benzene to ethylene. This ratio keeps the catalyst in use from being poisoned and thus ineffective. Since the ratio is 4.36:1 benzene to ethylene in the base case design, this ratio is kept for the optimized design as well. With the implementation of both the lower grade of benzene and the newer catalyst, the parallel design of reactor train continues in the optimized topology also. The controllability of feed rates and the temperature of our feed train leads to a positive impact and is an economically attractive improvement.

Figure 7, shown below, contains the optimized process flow diagram design. Table 4, further below, contains the respective stream tables for this optimized design.

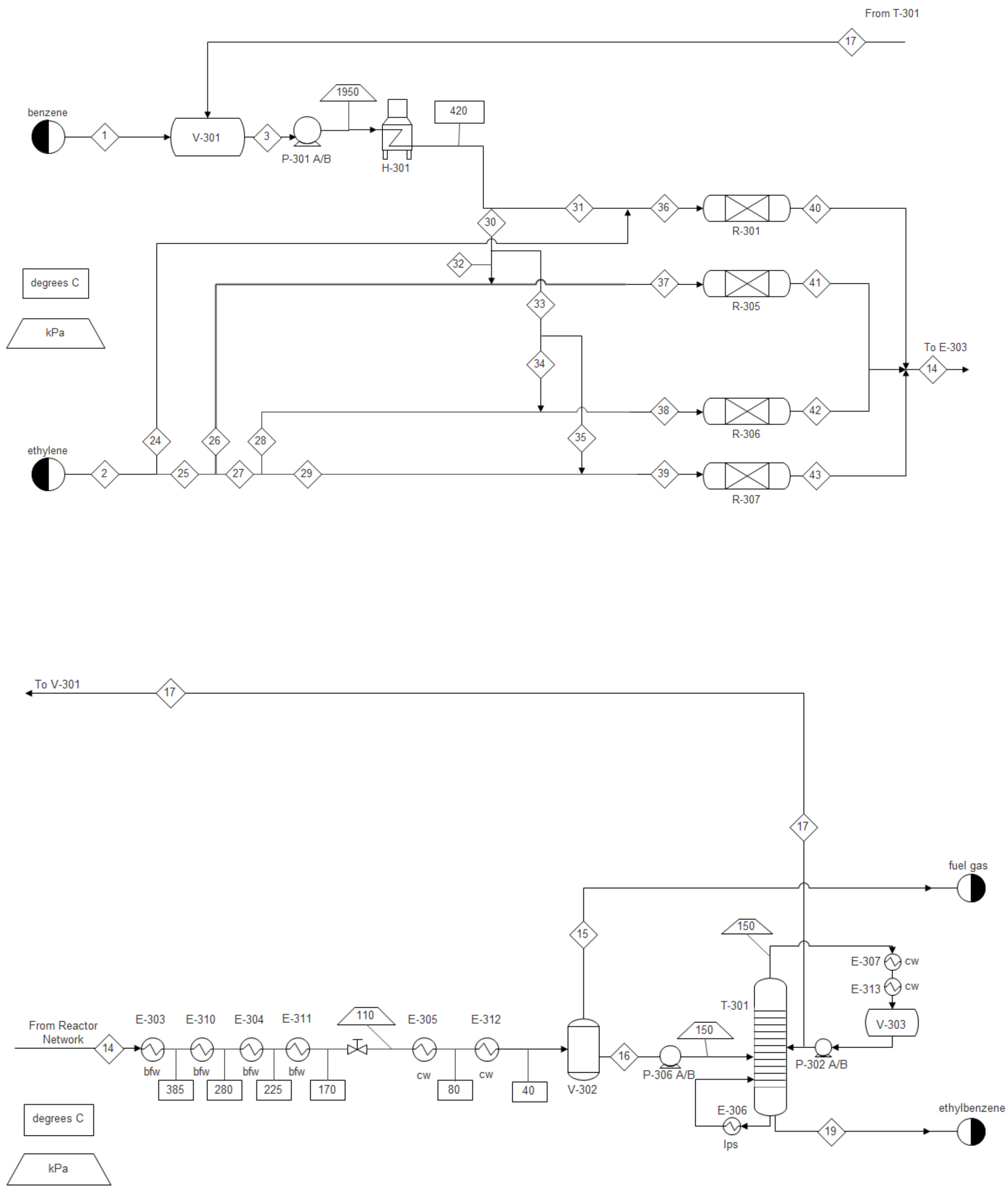


Figure 7 – Optimized case process flow diagram

Table 4 – Flow stream summary for the optimized ethylbenzene production plant

Stream Name	1	2	3	24	25	26
Temperature °C	25.0	25.0	38.6	25.0	25.0	25.0
Pressure kPa	110.0	2000.0	110.0	2000.0	2000.0	2000.0
Vapor Mole Fraction	0.0	1.0	0.0	1.0	1.0	1.0
Total kmol/h	93.4	102.9	475.6	25.7	77.2	25.7
Total kg/h	7426.0	2893.5	36557.3	723.4	2170.1	723.4
Flowrates in kmol/h						
Ethylene		99.83	0.0025	24.96	74.87	24.96
Ethane		3.09	1.69	0.77	2.32	0.77
Propylene			18.6			
Benzene	84.1		445.0			
Toluene	9.34		9.34			
Ethylbenzene			1.02			
1,4-DiEthBenzene						

Stream Name	27	28	29	30	31	32
Temperature °C	25.0	25.0	25.0	420.0	420.0	420.0
Pressure kPa	2000.0	2000.0	2000.0	1950.0	1950.0	1950.0
Vapor Mole Fraction	1.0	1.0	1.0	1.0	1.0	1.0
Total kmol/h	51.5	25.7	25.7	356.7	118.9	118.9
Total kg/h	1446.8	723.4	723.4	27418.0	9139.3	9139.2
Flowrates in kmol/h						
Ethylene	49.9	25.0	25.0	0.0	0.0	0.0
Ethane	1.54	0.772	0.772	1.267	0.422	0.422
Propylene				13.9	4.6	4.6
Benzene				333.7	111.2	111.2
Toluene				7.01	2.34	2.34
Ethylbenzene				0.762	0.254	0.254
1,4-DiEthBenzene						

Stream Name	33	34	35	36	37	38
Temperature ^{o}C	420.0	420.0	420.0	390.7	390.7	390.7
Pressure kPa	1950.0	1950.0	1950.0	1950.0	1950.0	1950.0
Vapor Mole Fraction	1.0	1.0	1.0	1.0	1.0	1.0
Total kmol/h	237.8	118.9	118.9	144.6	144.6	144.6
Total kg/h	18278.8	9139.4	9139.4	9862.7	9862.6	9862.8
Flowrates in kmol/h						
Ethylene	0.00124	0.00062	0.00062	25.0	25.0	25.0
Ethane	0.844	0.422	0.422	1.194	1.194	1.194
Propylene	9.28	4.64	4.64	4.64	4.64	4.64
Benzene	222.5	111.2	111.2	111.2	111.2	111.2
Toluene	4.67	2.34	2.34	2.34	2.34	2.34
Ethylbenzene	0.508	0.254	0.254	0.254	0.254	0.254
1,4-DiEthBenzene						

Stream Name	39	40	41	42	43
Temperature ^{o}C	390.7	489.5	489.5	489.5	489.5
Pressure kPa	1950.0	1522.9	1522.9	1522.9	1522.9
Vapor Mole Fraction	1.0	1.0	1.0	1.0	1.0
Total kmol/h	144.6	122.0	122.0	122.0	122.0
Total kg/h	9862.8	9862.7	9862.6	9862.8	9862.8
Flowrates in kmol/h					
Ethylene	25.0	0.00225	0.00225	0.00225	0.00225
Ethane	1.19	1.19	1.19	1.19	1.19
Propylene	4.64	6.97	6.97	6.97	6.97
Benzene	111.2	91.0	90.9	91.0	91.0
Toluene	2.34	0.000985	0.000985	0.000985	0.000985
Ethylbenzene	0.254	22.9	22.9	22.9	22.9
1,4-DiEthBenzene		1.9x10^-5	1.9x10^-5	1.9x10^-5	1.9x10^-5

Stream Name	14	15	16	17	19
Temperature °C	491.0	40.0	40.0	42.3	155.4
Pressure kPa	1935.0	110.0	110.0	150.0	165.0
Vapor Mole Fraction	1.0	1.0	0.0	0.0	0.0
Total kmol/h	488.0	15.2	472.8	382.2	90.6
Total kg/h	39450.8	705.2	38745.7	29132.8	9612.9
Flowrates in kmol/h					
Ethylene	0.00900	0.00652	0.00248	0.00248	
Ethane	4.78	3.09	1.69	1.69	
Propylene	27.9	9.3	18.6	18.6	
Benzene	363.8	2.7	361.1	360.9	0.2
Toluene	0.00394	0.00001	0.00393	0.00182	0.00211
Ethylbenzene	91.5	0.089	91.4	1.01	90.411
1,4-DiEthBenzene	7.5x10^-5		7.5x10^-5		7.5x10^-5

Economic Analysis of Optimized Design

A detailed economic analysis is necessary to optimize the objective function of the plant design improvement. The objective function in this research is to maximize the net present value.

The project length for the ethylbenzene plant is 12 years with a start-up time period 2 years before. The hurdle rate (MARR, after tax) is 12%.

A Chemical Engineering Plant Cost Index (CEPCI) is a composite index that accounts for inflation and the effects of time on the value of money [2]. CAPCOST is a program run in Microsoft Excel that estimates the value of equipment to determine the capital cost of a plant. A user must enter a CEPCI value to determine an accurate modern day capital cost. A CEPCI value of 587.4 is the most recent and reliable value for estimating the total cost for this plant. Obeying the economic parameters included in the base case study packet, the net present value for this optimized case design is $34.4 million.

There are many factors that affect the cost of manufacturing ethylbenzene. Table 5, seen below, contains the most important costs associated in the production of ethylbenzene. The important factors governing the day-to-day operation of this optimized plant are important to estimate the economic feasibility. A summary of the manufacturing costs, in units of dollars per time, gives an estimate for the practicality to operate the chemical process.

Table 5 – Summary of Cost of Manufacturing without Depreciation (COM_d)

Factors	Cost per year
Grass Roots	$12,500,000.00
Utilities	$1,169,464.18
Labor	$805,000.00
Raw Materials	$79,031,303.50
COM_d	$103,094,594.25

Table 6, below, summarizes the utility requirements for the equipment in the optimized ethylbenzene process. The steam generated from heat exchangers E-303, E-310, E-304, and E-311 count for credit towards the annual cost of utilities and positively impact the economic impact for this design. The prices for steam and cooling water are costs already associated with inefficiencies inherent in their use. It is assumed that an efficiency of 1 accounts for the full credit of their use. An efficiency of 0.8 in the fired heater, H-301, and an efficiency of 0.85 for pumps P-301 and P-306 take in to account inefficiencies of operation. [2]

Table 6 – Summary of Utility Requirements for the Equipment in the Ethylbenzene Production Process

Equipment	Utility	Duty (GJ/hr)	Efficiency	Price ($/GJ)	Annual Cost
E-303	High Pressure Steam	10.14	1	-17.7	-$1,493,616
E-310	High Pressure Steam	9.2	1	-17.7	-$1,355,154
E-304	Medium Pressure Steam	9.3	1	-14.83	-$1,147,762
E-311	Low Pressure Steam	10.4	1	-14.05	-$1,216,011
E-305	Cooling Water	4.4	1	0.354	$12,962
E-312	Cooling Water	5.9	1	0.354	$17,381
E-306	Low Pressure Steam	20.2	1	14.05	$2,361,867
E-307	Cooling Water	16.5	1	0.354	$48,609
E-313	Cooling Water	1.5	1	0.354	$4,419
H-301	Natural Gas	39.3	0.8	11.1	$4,537,883
P-301	Electricity	34.3	0.85	0.06	$20,149
P-302	Electricity	1	1	0.06	$499
P-306	Electricity	0.05	0.85	0.06	$29
T-301	n/a	n/a	n/a	n/a	n/a
V-301	n/a	n/a	n/a	n/a	n/a
V-302	n/a	n/a	n/a	n/a	n/a
V-303	n/a	n/a	n/a	n/a	n/a
R-301 (V-306)	n/a	n/a	n/a	n/a	n/a
R-305 (V-307)	n/a	n/a	n/a	n/a	n/a
R-306 (V-308)	n/a	n/a	n/a	n/a	n/a
R-307 (V-309)	n/a	n/a	n/a	n/a	n/a
			Total Cost of Utilities		$1,786,807

Table 7, below, contains the optimized fixed capital cost investment summary. A visualization of the percentage that each individual piece of equipment highlights the magnitude of the overall cost importance of the individual piece. Fixed capital costs are independent of changes in production rate. The costs are charged at the same rate even during periods when the plant is not in operation.

Table 7 – Summary of Fixed Capital Investment

Equipment	Bare Module Cost	Percentage of FCI
E-303	$177,000	1.8%
E-310	$288,000	2.9%
E-304	$269,000	2.7%
E-311	$128,000	1.3%
E-305	$103,000	1.0%
E-312	$86,500	0.9%
E-306	$666,000	6.7%
E-307	$153,000	1.5%
E-313	$115,000	1.1%
H-301	$3,980,000	39.8%
P-301	$203,000	2.0%
P-302	$28,200	0.3%
P-306	$32,900	0.3%
T-301	$538,000	5.4%
V-301	$194,000	1.9%
V-302	$90,300	0.9%
V-303	$38,500	0.4%
R-301 (V-306)	$730,000	7.3%
R-305 (V-307)	$730,000	7.3%
R-306 (V-308)	$730,000	7.3%
R-307 (V-309)	$730,000	7.3%
Total	$10,010,400	100

Table 8, below, summarizes the optimized case design. The optimized case summary is referenced many times in the description of the optimized case design in the following section and includes an organized table here for convenience to the reader. All calculations for the optimized case equipment come from CAPCOST. The user has to have knowledge of certain limitations on equipment to present reasonable data for the limitations. Guidelines for experience-based principles to input in to the CAPCOST program are used throughout the economic analysis [2].The materials of construction (MOC) used for the equipment throughout is carbon steel (CS) as a result of the low cost, availability and resistance to abrasion advantages comparted to other metal materials.

Table 8 – Optimized Case Equipment Summary

Exchangers	Type	Shell P (barg)	Tube P (barg)	MOC	Area (square meters)
E-303	Floating Head	41	18.4	CS/CS	182
E-310	Floating Head	41	18.4	CS/CS	368
E-304	Fixed	18.4	10	CS/CS	588
E-311	Fixed	18.4	5	CS/CS	131
E-305	Floating Head	18.4	3	CS/CS	58.2
E-312	Fixed	0.65	5	CS/CS	40.4
E-306	Floating Head	0.1	3	CS/CS	163
E-307	Floating Head	0.5	3	CS/CS	1000
E-313	Floating Head	0.5	3	CS/CS	89.9
Fired Heaters	**Type**	**Heat Duty (GJ/hr)**	**Pressure (barg)**	**MOC**	
H-301	Process Heater	49.2	18.5	CS	
Pumps	**Type**	**Power (kW)**	**# Spares**	**MOC**	**Discharge P (barg)**
P-301	Positive Displacement	40.4	1	CS	18.5
P-302	Centrifugal	1	1	CS	0.5
P-306	Positive Displacement	0.06	1	CS	0.5
Towers	**Type**	**Height (m)**	**Diameter (m)**	**MOC**	**Pressure (barg)**
T-301	26 Sieve Trays	17	2.75	CS	0.2
Vessels	**Orientation**	**Length/Height (m)**	**Diameter (m)**	**MOC**	**Pressure (barg)**
V-301	Vertical	8.1	2.7	CS	0.05
V-302	Vertical	5.7	1.9	CS	0.1
V-303	Horizontal	3	1	CS	0.05
R-301 (V-306)	Horizontal	10	2	CS	18.5
R-305 (V-307)	Horizontal	10	2	CS	18.5
R-306 (V-308)	Horizontal	10	2	CS	18.5
R-307 (V-309)	Horizontal	10	2	CS	18.5

Description of Optimized Design

A detailed description of the optimized design for theproduction of ethylbenzene is necessary to fully justify the improvements. An evaluation of each major section and the major changes involved follows.

Below, in Figure 8, is the first major section of the plant highlighting the two raw material feed inputs and the necessary optimized equipment to prepare the streams for the reactor train. A benzene feed (Stream 1) overall feed rate of 93.4 kmol/h and an ethylene feed (Stream 2) of 102.9 kmol/h meets the product specifications while maintaining a manageable raw material feed cost. The ethylene feed (Stream 2) splits in to four equal molar components to form Streams 24, 26, 28, and 29. These streams prepare for mixing with the four equal molar components of the combined benzene feed and recycle from T-301. These four mixed streams then enter the reactor train section. The ethylene feed (Stream 2) enters at a temperature of 25 °C and a pressure of 2000 kPa. The benzene feed (Stream 1) enters at a temperature of 25 °C and a pressure of 110 kPa and mixes with the recycle from T-301 (Stream 17) in V-301 to form stream 3. V-301 is a vertical vessel oriented to mix both the benzene feed and recycle streams. V-301 is sized at a height of 8.1 m with a diameter of 2.7 m and is made of carbon steel. Stream 3 is pumped to a pressure of 1950 kPa by P-301 A/B and increases to a reactor preparation temperature of 420 °C by way of the fired heater H-301. P-301 A/B has a duty of 34.3 GJ/h and is made of stainless steel to compensate for the higher process pressure. H-301 has a heat duty of 49.2 GJ/h and is made of stainless steel to account for both the high process temperature and pressure. The resulting stream is split in four equal molar portions similar to the ethylene feed splits in order to maintain the minimum reactor feed benzene to ethylene component ratio of 4.36:1. A ratio of 4.36:1 benzene to ethylene reactor feed ratio prevents catalyst poisoning while maintaining an effective reactor train conversion. Suppression of the diethylbenzene production and the additional side alkylation reactions occurs as well.

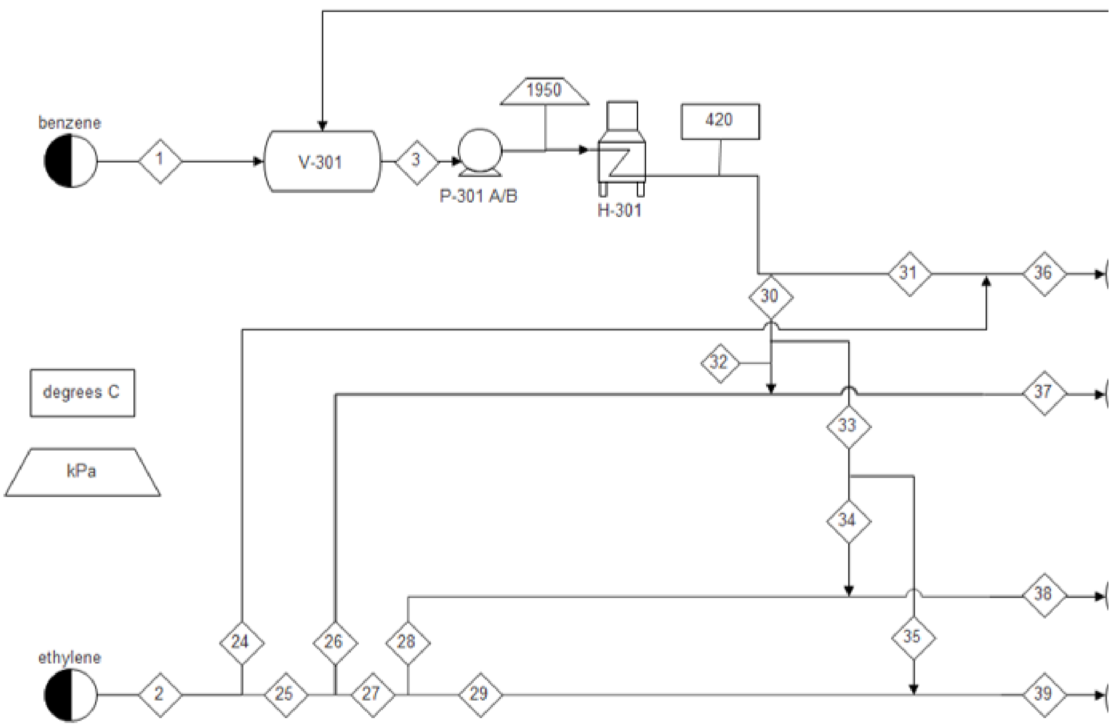


Figure 8 – Raw material feed and reactor feed preparation

The next major section of the optimized design is the reactor train section and Figure 9, below, gives a visual representation of the equipment and streams. The four equal molar components with the same 4.36:1 benzene to ethylene component feed ratiosenter each reactor in a parallel reactor design. Four identical reactors in parallel, sized at 10 m length and 2.11 m in diameter, adheres to the heuristic of a 5:1 reactor length to diameter ratio [2]. In each reactor, a 0.5 m space prevents waste of catalyst due to channeling of the streams in and out of each respective reactor. Each reactor is made of stainless steel to compensate for the high process temperature and pressure of the process streams by providing a safer inherent design. Streams 40-43 have identical component and overall flowrates as well as an identical reactor effluent temperature and pressure of 489.5 °C and 1522.9 kPa respectively. These four identical streams combine to form stream 14. Stream 14 continues to the heat exchanger network.

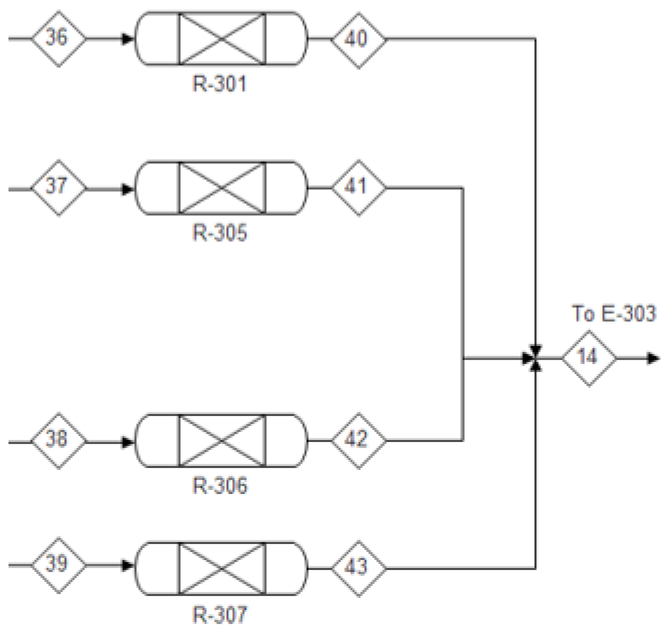


Figure 9 – Parallel Reactor Train

The third major section of the optimized design includes the heat exchanger network and the separation feed preparation sections. Figure 10, below, visualizes the necessary equipment in this section. Stream 14, at 491 °C, 1935 kPa,with an overall flowrate of 488 kmol/h, enters the heat exchanger network producing utilities to be sold to a sister styrene production plant. This network also adjusts the necessary separation feed temperature and pressure conditions. E-303 and E-310 produce high pressure steam that is sold for $17.7/GJ and they perform at duties of 10.14 GJ/h and 9.2 GJ/h respectively. The effluent from the first two heat exchangers has a temperature of 280 °C and is sent to E-304 having a duty of 9.3 GJ/h that produces medium pressure steam that sells for $14.83/GJ. The effluent from E-304 at a temperature of 225 °C is sent to E-311 having a duty of 10.4 GJ/h to produce low pressure steam that sells for $14.05/GJ. A pressure control valve reduces the pressure from 1950 kPa to 110 kPa to prepare the stream for the separation section. The vapor quality of the effluent stream from E-311 is not high enough to merit any more energy credit by way of an expander or turbine and it remains a liquid to be sent to the separation section without any more appreciable energy recovery consideration. The process stream continues through E-305 and E-312 each having duties of 4.4 GJ/h and 5.9 GJ/h respectively and each using cooling water as a cost for utilities to account for in the annual operating costs. The heat exchanger network effluent has a temperature of 40 °C and a pressure of 110 kPa. All of the heat exchangers in this network contain carbon steel for both the shell and tubes to minimize the fixed capital cost investment for our equipment. The effluent process stream, at a temperature of 40 °C, continues to the flash vaporizer (V-302) to minimize the loss of the raw material benzene in the overhead fuel gas. By circulating the benzene through the separation section and further on to the recycle stream and reactor train, more benzene reacts further to form even more ethylbenzene and thus enhances the net present value of the optimized design. The overhead fuel gas (Stream 15) continues to the fired heater as a side product and mostly contains the light gases of propylene and ethane. The condensed liquid (Stream 16) from the two-phase separator (V-302) at a temperature of 40 °C and a pressure of 110 kPa continues to a pump, P-306 A/B, to attain the separator feed pressure condition of 150 kPa.

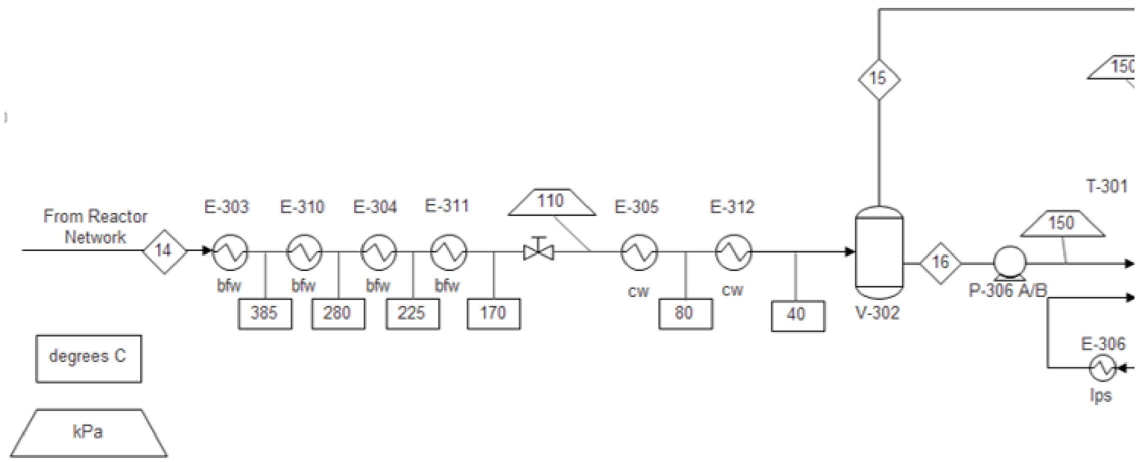


Figure 10 – Heat exchanger network and separation feed preparation

The final section in the optimized design, located below in Figure 11, composes the separation section and features a single distillation column, T-301. This section, also the most important and costly step in the plant, separates the ethylbenzene product at a purity of 99.8% ethylbenzene at a rate of 80,000 tonne/yr containing an impurity less than 2 ppm of diethylbenzene. The necessary flowrate of the product (Stream 19) is a design constraint of the rigorous column implemented in PRO/II. The distillation column, T-301, operates with an efficiency of 75% and has a heuristic safety factor of 1.1 incorporated in the sizing calculations for tray spacing considerations. The number of actual trays needed is 26 sieve trays. 3 meters of height adds to the overall height as well to result in an overall height of 17 meters. A diameter of 2.75 meters maintains the length to diameter ratio heuristic between values of 30 and 2 meters. The feed to T-301 has a temperature of 40 °C and a pressure of 110 kPa. The light component is benzene and the heavy component is ethylbenzene for this separation. The top tray pressure ofT-301 is 150 kPa and the bottom tray pressure is 165 kPa, therefore, the pressure drop across the column is 15 kPa or 0.15 bar. The reboiler, E-306, uses low pressure steam as a utility and performs at a duty of 20.2 GJ/h. The limitations for area in square meters in CAPCOST for heat exchangers is 1000 m^2, therefore, the condenser for T-301 had to be modeled as two separate condensers E-307 and E-313 which have duties of 16.5 GJ/h and 1.5 GJ/h respectively. V-303 is a horizontal vessel sized at a length of 4.05 m and a height of 1.35 m. V-303 is made of carbon steel. The final part of the total condenser of T-301 is P-302 A/B which pumps both the liquid reflux back in to the top of T-301 and the total liquid phase top product (Stream 17). The liquid product recycles back to V-301 and maintains a pressure of 150 kPa. P-302 A/B is made of carbon steel.

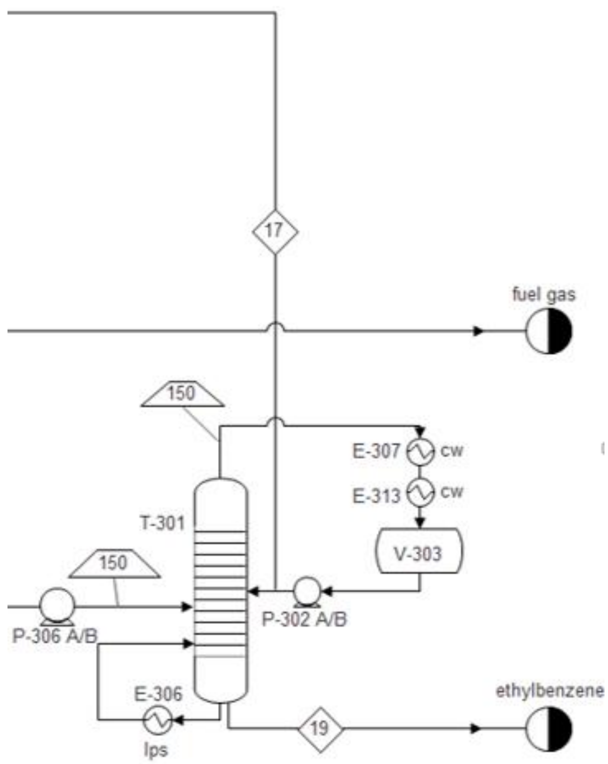


Figure 11 – Separation section

Conclusion

A detailed analysis of the given case study base gives a focused starting point to an optimization problem. This analysis leads to a justified and optimized design for a new and improved ethylbenzene plant. Elimination of several pieces of equipment as well as certain utilities that are costly aid in the minimizing the final EAOC value and subsequently maximizing the net present value (NPV). Both the addition of the newer catalyst proposed and the cheaper benzene feed stream positively impact the economic growth of the plant as well. A net present value of $34.4 million results. The proposed changes are justified and are recommended in order to optimize the design.

Recommendations

A first recommendation involves decreasing the overall flowrate throughout the process design with a predominant focus the recycle section.

Another recommendation involves further investigating the catalyst poisoning possibilities of the catalyst in use in the reactor train. The benzene to ethylene feed ratio to each reactor was maintained at a relatively high number starting at 8:1 with a minimum of 4.36:1 in the base case to both combat the catalyst poisoning as well as to suppress the production of diethylbenzene. More research in to this phenomenon leads to a better understanding of the optimum feed ratios needed for each reactor feed to better improve the production of ethylbenzene to possibly reduce the raw material feed costs.

Process Safety

The temperature and pressure limits of the vessels in use for this plantis a first concern. To avoid uncontrolled, catastrophic releases of chemicals and/or destruction of process vessels, vessels contain pressure-relief systems, which open automatically when the pressure reaches a specified limit. Tanks and pressure-relief systems require regular inspection to ensure integrity.

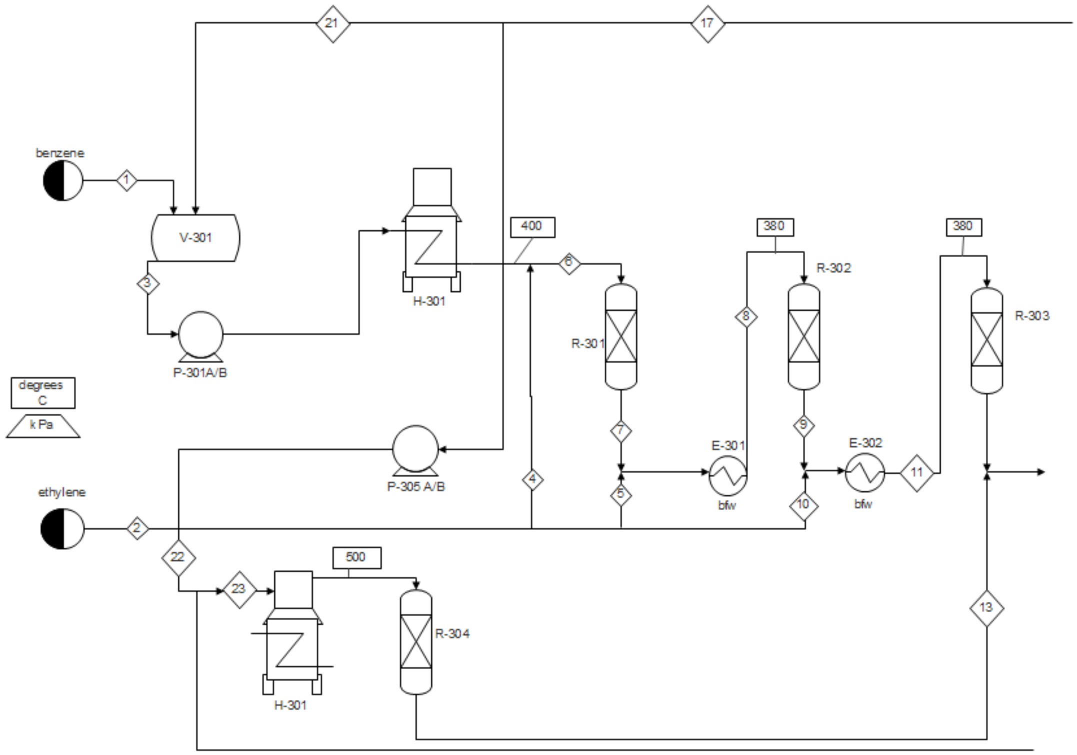
Ethylene, benzene, and ethylbenzene are all flammable, and plans of action develop in case of a fire. Gas detectors exist throughout the plant in order to monitor the composition of air and ensure the chemicals in the air do not reach the lower flammability limit. Additionally, chemicals and potential sources of leaks are all kept away from potential sources of ignition. In the event of a fire, firefighters use dry chemical powder to extinguish small fires and alcohol foam, water spray, or fog for large fires. Firefighters wear self-contained breathing apparatuses and full turnout gear.

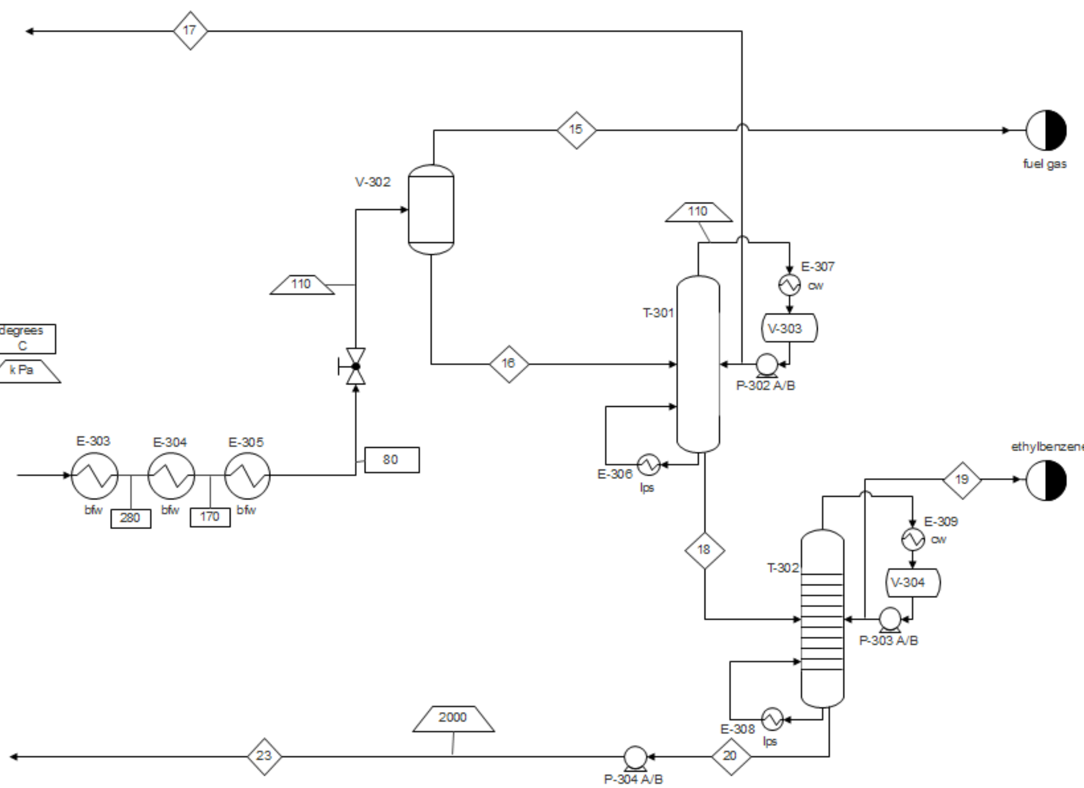
Workers wear splash goggles, chemical suits, and respirators when there is any risk for inhalation of or exposure to the chemicals. Eye-wash stations must exist throughout the plant as well.

Permits for emissions are in effect prior to the construction of the plant and require modification and renewal should the plant undergo significant modification. These permits go through the state environmental protection agency and adhere to federal regulations. Process upsetsresult in emergency releases, in which case a control and response plan is in place dictating the protocol for the containment, removal, and disposal of any and all waste created in the process.

APPENDICES

Appendix A: Base Case PFD





Appendix B: Base Case Stream Tables

Stream Name	1	2	3	4	5
Temperature ^{o}C	25.0	25.0	17.1	25.0	25.0
Pressure kPa	110.0	2000.0	105.0	2000.0	2000.0
Vapor Mole Fraction	0.0	1.0	0.0	1.0	1.0
Total kmol/h	89.3	100.0	239.9	30.0	35.0
Total kg/h	7011.4	2819.5	18633.5	845.8	986.8
Flowrates in kmol/h					
Ethylene		93.0	1.19	27.9	32.55
Ethane		7.00	1.11	2.10	2.45
Propylene			1.24		
Benzene	86.6		233.02		
Toluene	2.68		2.68		
Ethylbenzene			0.620		
1,4-DiEthBenzene			9.13x10^-8		

Stream Name	6	7	8	9	10
Temperature ^{o}C	383.2	429.4	380.0	441.2	25.0
Pressure kPa	2000.0	1985.0	1960.0	1960.0	2000.0
Vapor Mole Fraction	1.0	1.0	1.0	1.0	1.0
Total kmol/h	269.9	249.8	284.8	256.2	35.0
Total kg/h	19479.3	19479.3	20466.1	20466.1	986.8
Flowrates in kmol/h					
Ethylene	29.1	6.48	39.0	10.3	32.6
Ethane	3.21	3.21	5.66	5.66	2.45
Propylene	1.24	3.79	3.79	3.92	
Benzene	233.0	215.5	215.5	187.1	
Toluene	2.68	0.1372	0.1372	7.13x10^-5	
Ethylbenzene	0.6203	20.7	20.7	49.3	
1,4-DiEthBenzene	9.13x10^-8	0.0022	0.0022	0.0122	

Stream Name	**11**	**12**	**13**	**14**	**15**
Temperature ^{o}C	380.0	442.4	500.0	450.6	73.6
Pressure kPa	1935.0	1935.0	2000.0	1935.0	198.3
Vapor Mole Fraction	1.0	1.0	1.0	1.0	1.0
Total kmol/h	291.2	260.2	46.9	307.1	29.5
Total kg/h	21453.0	21453.0	3673.1	25126.0	1375.4
Flowrates in kmol/h					
Ethylene	42.9	11.9	0.0137	11.9	10.3
Ethane	8.11	8.11	0.3397	8.45	7.00
Propylene	3.92	3.92	0.3824	4.31	2.68
Benzene	187.1	156.1	44.60	200.7	8.8910217
Toluene	7.13x10^-5	2.20x10^-9	9.55x10^-11	2.29x10^-9	3.78x10^-11
Ethylbenzene	49.3	80.2	1.53	81.72	0.6398
1,4-DiEthBenzene	0.0122	0.0310	0.0013	0.0323	4.58E-05

Stream Name	**16**	**17**	**18**	**19**	**20**
Temperature ^{o}C	73.6	12.3	142.7	139.3	150.1
Pressure kPa	198.3	105.0	120.0	110.0	140.0
Vapor Mole Fraction	0.0	0.0	0.0	0.0	0.0
Total kmol/h	277.6	196.8	91.5	90.6	1.0
Total kg/h	23750.6	15193.3	9714.0	9612.1	101.9
Flowrates in kmol/h					
Ethylene	1.56	1.56			
Ethane	1.45	1.45			
Propylene	1.63	1.63			
Benzene	191.8	191.4	0.2058	0.2056	0.000213
Toluene	2.25x10^-9	3.9x10^-10	2.06x10^-9	2.06x10^-9	5.29X10^-12
Ethylbenzene	81.08	0.8109	91.30	90.39	0.9131
1,4-DiEthBenzene	0.0323	1.19x10^-7	0.0367	3.67x10^-6	0.0367

Stream Name	21	22	23
Temperature ^{o}C	12.3	12.6	16.5
Pressure kPa	105.0	2000.0	2000.0
Vapor Mole Fraction	0.0	0.0	0.0
Total kmol/h	150.6	46.3	47.2
Total kg/h	11622.1	3571.2	3673.1
Flowrates in kmol/h			
Ethylene	1.19	0.3664	0.3664
Ethane	1.11	0.3397	0.3397
Propylene	1.24	0.3824	0.3824
Benzene	146.4	45.0	45.0
Toluene	2.98x10^-10	9.16x10^-11	9.69x10^-11
Ethylbenzene	0.6203	0.1906	1.10
1,4-DiEthBenzene	9.13x10^-8	2.81x10^-8	0.0367

Appendix C: Base Case Cash Flow Statement

Income Statement														
End of Year	1	2	3	4	5	6	7	8	9	10	11	12	13	14
Revenue			$112,878,926.53	$112,878,926.53	$112,878,926.53	$112,878,926.53	$112,878,926.53	$112,878,926.53	$112,878,926.53	$112,878,926.53	$112,878,926.53	$112,878,926.53	$112,878,926.53	$112,878,926.53
		$9,390,000	$8,048,169.00	$5,748,558.00	$4,106,247.00	$2,933,436.00	$2,094,909.00	$1,257,321.00	$418,794.00	$0.00	$0.00	$0.00	$0.00	$0.00
Expenses														
Materials			$85,410,532	$85,410,532	$85,410,532	$85,410,532	$85,410,532	$85,410,532	$85,410,532	$85,410,532	$85,410,532	$85,410,532	$85,410,532	$85,410,532
Labor			$862,500	$888,375	$915,026	$942,477	$970,751	$999,874	$1,029,870	$1,060,766	$1,092,589	$1,125,367	$1,159,128	$1,193,902
Utilities			$2,103,985	$2,103,985	$2,103,985	$2,103,985	$2,103,985	$2,103,985	$2,103,985	$2,103,985	$2,103,985	$2,103,985	$2,103,985	$2,103,985
Catalyst		$276,012			$276,012			$276,012			$276,012			
Others			$22,858,864	$22,903,628	$22,949,734	$22,997,224	$23,046,139	$23,096,521	$23,148,414	$23,201,865	$23,256,918	$23,313,624	$23,372,030	$23,432,189
Depreciation			0.1429	0.2449	0.1749	0.1249	0.0893	0.0892	0.0893	0.0446				
Building			$1,341,831	$2,299,611	$1,642,311	$1,172,811	$838,527	$837,588	$838,527	$418,794	$0	$0	$0	$0
Machines			$0.00	$0.00	$0.00	$0.00	$0.00	$0.00	$0.00	$0.00				
Tools														
Taxable Income			$301,214	-$727,205	-$142,662	$251,897	$508,992	$430,426	$347,598	$682,984	$1,014,902	$925,419	$833,251	$738,319
Income Taxes			$135,546	-$327,242	-$64,198	$113,354	$229,046	$193,692	$156,419	$307,343	$456,706	$416,438	$374,963	$332,243
Net Income			$165,668	-$399,963	-$78,464	$138,543	$279,946	$236,735	$191,179	$375,641	$558,196	$508,980	$458,288	$406,075
Cash Flow Statement														
Operating Activities														
Net Income			$165,668	-$399,963	-$78,464	$138,543	$279,946	$236,735	$191,179	$375,641	$558,196	$508,980	$458,288	$406,075
Depreciation			$1,341,831	$2,299,611	$1,642,311	$1,172,811	$838,527	$837,588	$838,527	$418,794	$0	$0	$0	$0
Investment Activities														
Land														
Buildings	$5,634,000	-$3,756,000												
Machines	$0.00	$0												
Tools														
Gains Tax														
Land														-$422,550
Buildings														$0
Machines														$939,000
Tools														
Working Capital		-$14,450,713.69	-$6,468.75	-$6,662.81	-$6,862.70	-$7,068.58	-$7,280.64	-$7,499.05	-$7,724.03	-$7,955.75	-$8,194.42	-$8,440.25	-$8,693.46	$14,533,564.12
Net Cash Flow	-$5,634,000.00	-$18,482,725.69	$1,501,030.05	$1,892,985.68	$1,556,983.94	$1,304,285.70	$1,111,191.97	$1,066,823.51	$1,021,981.76	$786,479.69	$550,001.51	$500,540.00	$449,594.64	$15,456,089.30
Cummulative Cash Flow	-$5,634,000.00	-$24,116,725.69	-$22,615,695.64	-$20,722,709.96	-$19,165,726.02	-$17,861,440.31	-$16,750,248.34	-$15,683,424.84	-$14,661,443.08	-$13,874,963.38	-$13,324,961.87	-$12,824,421.88	-$12,374,827.24	$3,081,262.06
Present Value	-$5,030,357.14	-$14,734,315.76	$1,068,403.54	$1,203,026.62	$883,474.50	$660,791.73	$502,646.82	$430,872.12	$368,536.87	$253,225.41	$158,112.29	$128,476.15	$103,035.49	$3,162,622.10
Cumul Discounted CF	-$5,030,357.14	-$19,764,672.91	-$18,696,269.36	-$17,493,242.74	-$16,609,768.24	-$15,948,976.51	-$15,446,329.69	-$15,015,457.57	-$14,646,920.70	-$14,393,695.29	-$14,235,583.00	-$14,107,106.85	-$14,004,071.36	-$10,841,449.27
Net Present Value														
MARR(12%) ($10,841,449.27)														

Appendix D: Equipment Sizing Calculations

Distillation Column:

In order to size the distillation columns appropriately, several calculations were necessary. Those calculations were carried out for both the distillate and bottoms streams, in the following order: stream densities, volumetric flow of the streams, linear velocities of the streams, and the diameter of the column required to sufficiently separate and transport each stream. The height must also be calculated. An example calculation is provided below.

First the density was calculated using the mass and vapor volumetric flows of the distillate and bottmos streams.

$$m_D := 29114.9\ \frac{kg}{hr} \qquad V_{Dv} := 9046.2\ \frac{m^3}{hr}$$

$$\rho_D := \frac{m_D}{V_{Dv}} \qquad \rho_D = 3.218\ \frac{kg}{m^3}$$

$$m_B := 9612.9\ \frac{kg}{hr} \qquad V_{Bv} := 2146.2\ \frac{m^3}{hr}$$

$$\rho_B := \frac{m_B}{V_{Bv}} \qquad \rho_B = 4.479\ \frac{kg}{m^3}$$

Next the total volumetric flow was calculated using the mass flows of the liquid and the previously calculated densities. The reflux ratio of the condenser was also used in calculating the distillate volumetric flow rate to account for both liquid and vapor volumetric flows.

$$R := .602 \qquad m_{Dl} := 8232.1\ \frac{kg}{hr}$$

$$V_D := (1+R)\cdot\left(\frac{m_{Dl}}{\rho_D}\right) \qquad V_D = \left(4.098\cdot 10^3\right)\ \frac{m^3}{hr}$$

$$m_{Bl} := 61424.1\ \frac{kg}{hr}$$

$$V_B := \frac{m_{Bl}}{\rho_B} \qquad V_B = \left(1.371\cdot 10^4\right)\ \frac{m^3}{hr}$$

After that, the linear velocities of both the distillate and bottoms streams were calculated using the stream densities previously found and the vapor factor of 1.35 m/s*(kg/m^3)$^{.5}$ was used, falling between the values of 1.2 and 1.5 m/s*(kg/m^3)$^{.5}$ recognized by Turton et al. as the upper and lower limits respectively for an economically efficient distillation column.

$$v_D := \frac{1.35\ \frac{m}{s}\cdot\left(\frac{kg}{m^3}\right)^{.5}}{\left(\rho_D^{\ .5}\right)} \qquad v_D = 0.753\ \frac{m}{s}$$

$$v_B := \frac{1.35\ \frac{m}{s}\cdot\left(\frac{kg}{m^3}\right)^{.5}}{\left(\rho_B^{\ .5}\right)} \qquad v_B = 0.638\ \frac{m}{s}$$

With the volumetric flows and linear velocities of the distillate and bottoms streams calculated, it became possible to calculate the required diameters of the distillate and bottoms streams, thus providing an appropriate diameter for the distillation column.

$$D_D := \left(\frac{4 \cdot V_D}{\pi \cdot v_D \cdot 3600 \, \frac{s}{hr}} \right)^{.5} \qquad D_D = 1.388 \ m$$

$$D_B := \left(\frac{4 \cdot V_B}{\pi \cdot v_B \cdot 3600 \, \frac{sec}{hr}} \right)^{.5} \qquad D_B = 2.757 \ m$$

Lastly, the height of the distillation column was calculated. This calculation required several assumptions to be made. The first was a tray efficiency of .75, a value falling between the values .6 and .9. The second assumption was that each tray requires half a meter in spacing. Next it was assumed that an additional 10% of column height would be required as a safety factor. The last assumption was that an additional 1.2 and 1.3 meters would be required for vapor disengagement at the top and bottom of the column respectively. These assumptions were based off of the recommendations made by Turton et al.

$$N_{theoretical} := 19 \qquad \varepsilon := .75$$

$$H := \left(\left(\frac{N_{theoretical}}{\varepsilon} \right) \cdot .5m \right) \cdot 1.1 + 3 \ m \qquad H = 16.933 \ m$$

Vessels:

In order to properly size the vessels throughout the ethylbenzene production process several calculations had to be carried out. Those calculations included volumetric flow rates of the feed streams into the vessels, holdup times, vessel volumes, and vessel heights and diameters. An example calculation is provide below.

First it was necessary to calculate the volumetric flow rate of the feed into each stream.

$$m := 36597.8\ \frac{kg}{hr} \qquad \rho := 846.1\ \frac{kg}{m^3}$$

$$V := \frac{m}{\rho} \qquad V = 43.255\ \frac{m^3}{hr}$$

Once the volumetric flow rate into each vessel was found it was possible to calculate the holdup time required for each vessel. For reflux drums the holdup time is 5 minutes, for drums feeding a tower the holdup time is 10 minutes and for drums feeding furnaces and fired heaters the holdup time is 30 minutes as recommended by Turton et al. The following calculation is for a drum feeding a furnace, thus the holdup time is 30 minutes. From the holdup time, the Solver function in Microsoft Excel was used to find the volume of the vessels.

$$t := \frac{\left(.5 \cdot Vol \cdot 60\ \frac{min}{hr}\right)}{V} \qquad t = 30\ min$$

$$Vol := 43.255\ m^3$$

Once the volume of the vessels was found, the height and diameter of the vessels could be found. This was done by using the optimum height to diameter ratio of 3 as recommended by Turton et al. and using the Solver function in Microsoft Excel.

$$k := \frac{H}{D} \qquad k = 3$$

$$H := 7.91\ m \qquad D := 2.637\ m$$

Heat Exchangers:

In order to properly size the heat exchangers in the ethylbenzene production process several calculations were carried out. Those calculations included the mass flow rate of the water, latent and sensible heats, intermediate temperature of the process stream, log mean temperatures of both the latent and sensible portions of the exchanger, latent and sensible heat exchanger areas and total heat exchanger area. It is important to note that when no phase change occurs in the water, only the sensible heat exchanger calculations were and when only a phase change occurs, only the latent heat exchanger calculations were performed. An example equation is provided below for a heat exchanger experiencing both latent and sensible heat transfer.

First the mass of the water required in the heat exchanger had to be calculated.

$T_{pf} := 225\ °C \qquad T_{pe} := 170\ °C$

$T_{wf} := 115\ °C \qquad T_{wm} := 160\ °C \qquad T_{we} := 160\ °C$

$Q_t := 287888.9\ W$

$H_{wf} := 485400\ \frac{J}{kg} \qquad H_{wm} := 678960\ \frac{J}{kg} \qquad H_{we} := 2757625\ \frac{J}{kg}$

$m_w := \frac{Q_t}{H_{we} - H_{wf}} \qquad m_w = 0.127\ \frac{kg}{s}$

Once the mass of the water was obtained, it was possible to calculate both the latent and sensible heats.

$$Q_l := m_w \cdot \left(H_{we} - H_{wm}\right) \qquad Q_l = \left(2.634 \cdot 10^5\right)\ \boldsymbol{W}$$

$$Q_s := m_w \cdot \left(H_{wm} - H_{wf}\right) \qquad Q_s = \left(2.452 \cdot 10^4\right)\ \boldsymbol{W}$$

With the sensible and latent heats calculated, the intermediate process stream temperature was calculated.

$$T_{pm} := \left(\frac{Q_l}{Q_t}\right) \cdot \left(T_{pe} - T_{pf}\right) + T_{pf} \qquad T_{pm} = 174.685\ \boldsymbol{°C}$$

The log mean temperature difference, the driving force behind the heat transfer, could then be calculated for both sensible and latent heat transfer areas. It was assumed that the maximum log mean temperature difference was 100 K as recommended by Turton et al.

$$T_{LMl} := \frac{\left(T_{pf} - T_{we}\right) - \left(T_{pm} - T_{wm}\right)}{\ln\left(\frac{\left(T_{pf} - T_{we}\right)}{\left(T_{pm} - T_{wm}\right)}\right)} \qquad T_{LMl} = 33.824\ \boldsymbol{K}$$

$$T_{LMs} := \frac{\left(T_{pm} - T_{wm}\right) - \left(T_{pe} - T_{wf}\right)}{\ln\left(\frac{\left(T_{pm} - T_{wm}\right)}{\left(T_{pe} - T_{wf}\right)}\right)} \qquad T_{LMs} = 30.53\ \boldsymbol{K}$$

After the log mean temperatures were calculated the latent and sensible areas were found, the sum of which was the total area of the heat exchanger. For the area of the sensible heat a fouling factor of 0.9 was assumed to account for inefficiencies in the heat transfer over time. It was also assumed that the maximum total area was 1000 m^3 for an economically practical heat exchanger as recommended by Turton et al.

$$U_l := 60 \frac{W}{m^2 \cdot K} \qquad U_s := 850 \frac{W}{m^2 \cdot K}$$

$$A_l := \frac{Q_l}{U_l \cdot T_{LMl}} \qquad A_l = 129.772\ m^2$$

$$A_s := \frac{Q_s}{U_s \cdot T_{LMs} \cdot .9} \qquad A_s = 1.05\ m^2$$

$$A_t := A_l + A_s \qquad A_t = 130.822\ m^2$$

Reactors:

In order to properly size the reactors in the ethylbenzene production process, it was necessary to do several calculations. These calculations were based on the catalyst length and volume and included the reactor diameter, length and volume. An assumed length to diameter ratio of about 5 was used with a maximum length of 10 meters as recommended by Turton et al. for horizontal vessels. An example calculation is provided below.

The diameter of the reactors was first calculated.

$$V_c := 31.47\ m^3 \qquad L := 9\ m$$

$$D := \left(\frac{V_c}{L \cdot \pi}\right)^{.5} \cdot 2 \qquad D = 2.11\ m$$

From the diameter, a volume could be calculated based on a length of 10 meters.

$$L_R := L + 1\ m \qquad L_R = 10\ m$$

$$V_R := \pi \cdot \left(\frac{D}{2}\right)^2 \cdot L_R \qquad V_R = 34.967\ m^3$$

Pumps:

To properly size the pumps in the ethylbenzene production process, several calculations had to be performed. These calculations included the volumetric flow rate through the pump, the pressure rise across the pump, and the power used by the pump. An example calculation is provided below.

First the volumetric flow into the pump was calculated.

$$m := 38727.8\ \frac{kg}{hr} \qquad \rho := 843.5\ \frac{kg}{m^3}$$

$$V := \frac{m}{\left(60\ \frac{min}{hr} \cdot \rho\right)} \qquad V = 0.765\ \frac{m^3}{min}$$

Next, the pressure rise across the pump was calculated.

$$P_f := 1.1\ bar \qquad P_e := 1.5\ bar$$

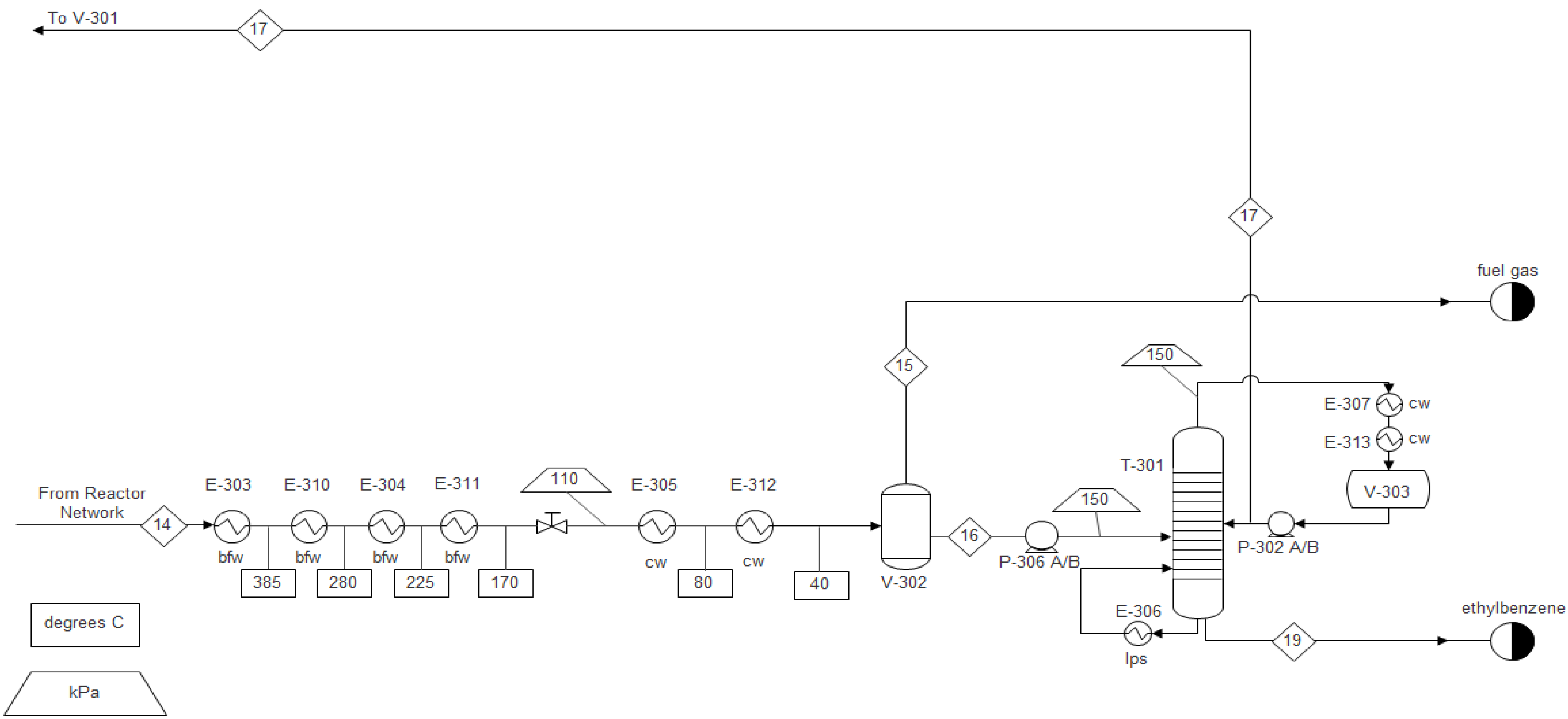
$$\Delta P := P_e - P_f \qquad \Delta P = 0.4\ bar$$

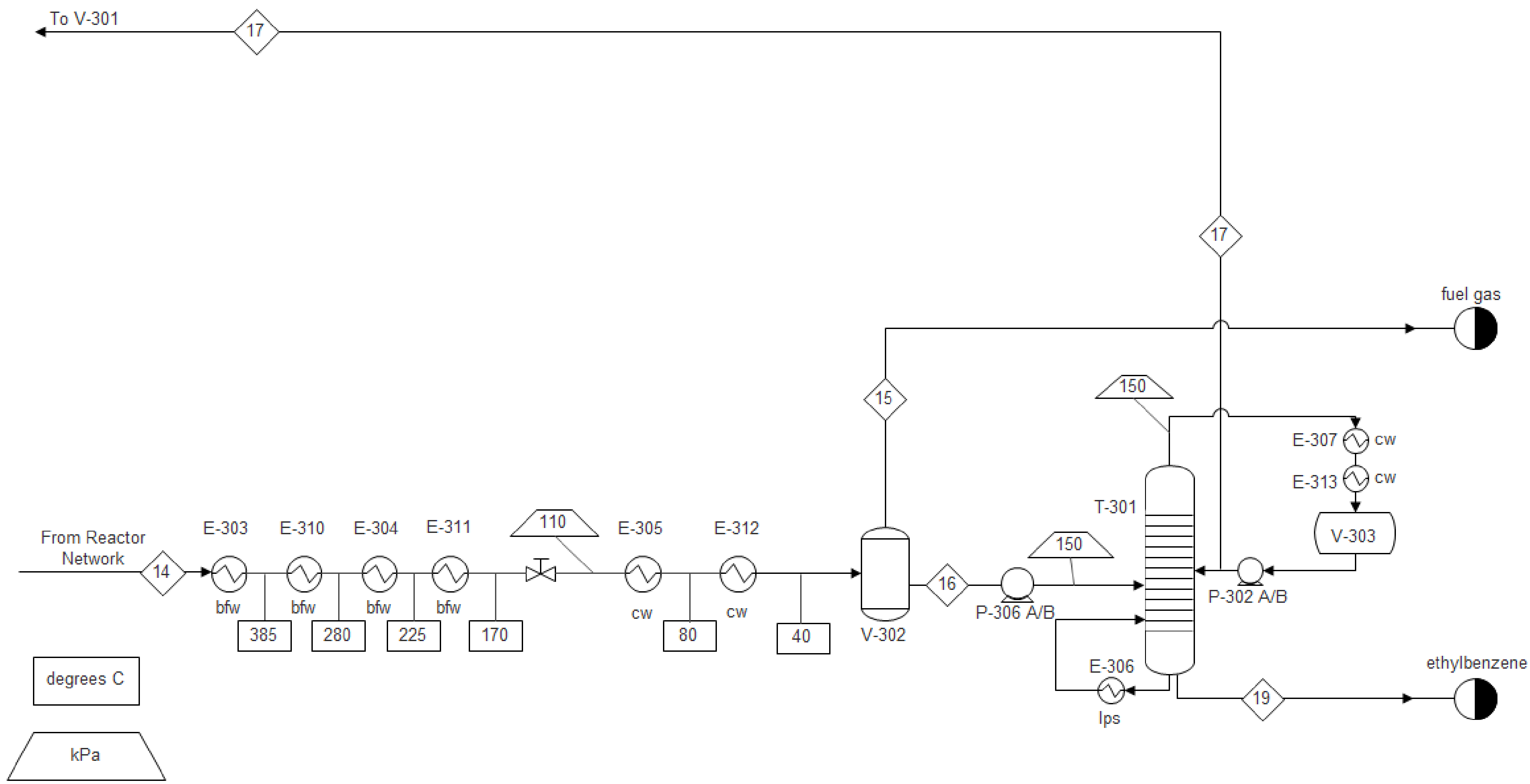
Last, the power required by the pump was calculated using the volumetric flow rate into the pump and pressure rise from the previous calculations. A pump efficiency of .8 was used as it falls in the middle of the efficiency range recommended by Turton et al.

$$\varepsilon := .8$$

$$W := \frac{(V \cdot \Delta P)}{\varepsilon} \qquad W = 0.638\ kW$$

Appendix E: Optimized PFD




To V-301
17
17
fuel gas
15
150
E-307
cw
E-313
cw
T-301
V-303
From Reactor Network
14
E-303
E-310
E-304
E-311
110
E-305
E-312
bfw
bfw
bfw
bfw
385
280
225
170
cw
80
cw
40
V-302
16
150
P-306 A/B
P-302 A/B
E-306
lps
19
ethylbenzene
degrees C
kPa

Appendix F: Optimized Stream Tables

Stream Name	1	2	3	24	25	26
Temperature ^oC	25.0	25.0	38.6	25.0	25.0	25.0
Pressure kPa	110.0	2000.0	110.0	2000.0	2000.0	2000.0
Vapor Mole Fraction	0.0	1.0	0.0	1.0	1.0	1.0
Total kmol/h	93.4	102.9	475.6	25.7	77.2	25.7
Total kg/h	7426.0	2893.5	36557.3	723.4	2170.1	723.4
Flowrates in kmol/h						
Ethylene		99.83	0.0025	24.96	74.87	24.96
Ethane		3.09	1.69	0.77	2.32	0.77
Propylene			18.6			
Benzene	84.1		445.0			
Toluene	9.34		9.34			
Ethylbenzene			1.02			
1,4-DiEthBenzene						

Stream Name	27	28	29	30	31	32
Temperature ^oC	25.0	25.0	25.0	420.0	420.0	420.0
Pressure kPa	2000.0	2000.0	2000.0	1950.0	1950.0	1950.0
Vapor Mole Fraction	1.0	1.0	1.0	1.0	1.0	1.0
Total kmol/h	51.5	25.7	25.7	356.7	118.9	118.9
Total kg/h	1446.8	723.4	723.4	27418.0	9139.3	9139.2
Flowrates in kmol/h						
Ethylene	49.9	25.0	25.0	0.0	0.0	0.0
Ethane	1.54	0.772	0.772	1.267	0.422	0.422
Propylene				13.9	4.6	4.6
Benzene				333.7	111.2	111.2
Toluene				7.01	2.34	2.34
Ethylbenzene				0.762	0.254	0.254
1,4-DiEthBenzene						

Stream Name	33	34	35	36	37	38
Temperature ^{o}C	420.0	420.0	420.0	390.7	390.7	390.7
Pressure kPa	1950.0	1950.0	1950.0	1950.0	1950.0	1950.0
Vapor Mole Fraction	1.0	1.0	1.0	1.0	1.0	1.0
Total kmol/h	237.8	118.9	118.9	144.6	144.6	144.6
Total kg/h	18278.8	9139.4	9139.4	9862.7	9862.6	9862.8
Flowrates in kmol/h						
Ethylene	0.00124	0.00062	0.00062	25.0	25.0	25.0
Ethane	0.844	0.422	0.422	1.194	1.194	1.194
Propylene	9.28	4.64	4.64	4.64	4.64	4.64
Benzene	222.5	111.2	111.2	111.2	111.2	111.2
Toluene	4.67	2.34	2.34	2.34	2.34	2.34
Ethylbenzene	0.508	0.254	0.254	0.254	0.254	0.254
1,4-DiEthBenzene						

Stream Name	39	40	41	42	43
Temperature ^{o}C	390.7	489.5	489.5	489.5	489.5
Pressure kPa	1950.0	1522.9	1522.9	1522.9	1522.9
Vapor Mole Fraction	1.0	1.0	1.0	1.0	1.0
Total kmol/h	144.6	122.0	122.0	122.0	122.0
Total kg/h	9862.8	9862.7	9862.6	9862.8	9862.8
Flowrates in kmol/h					
Ethylene	25.0	0.00225	0.00225	0.00225	0.00225
Ethane	1.19	1.19	1.19	1.19	1.19
Propylene	4.64	6.97	6.97	6.97	6.97
Benzene	111.2	91.0	90.9	91.0	91.0
Toluene	2.34	0.000985	0.000985	0.000985	0.000985
Ethylbenzene	0.254	22.9	22.9	22.9	22.9
1,4-DiEthBenzene		1.9x10^-5	1.9x10^-5	1.9x10^-5	1.9x10^-5

Stream Name	14	15	16	17	19
Temperature ^{o}C	491.0	40.0	40.0	42.3	155.4
Pressure kPa	1935.0	110.0	110.0	150.0	165.0
Vapor Mole Fraction	1.0	1.0	0.0	0.0	0.0
Total kmol/h	488.0	15.2	472.8	382.2	90.6
Total kg/h	39450.8	705.2	38745.7	29132.8	9612.9
Flowrates in kmol/h					
Ethylene	0.00900	0.00652	0.00248	0.00248	
Ethane	4.78	3.09	1.69	1.69	
Propylene	27.9	9.3	18.6	18.6	
Benzene	363.8	2.7	361.1	360.9	0.2
Toluene	0.00394	0.00001	0.00393	0.00182	0.00211
Ethylbenzene	91.5	0.089	91.4	1.01	90.411
1,4-DiEthBenzene	7.5x10^-5		7.5x10^-5		7.5x10^-5

Appendix G: Optimized Cash Flow Statement

Income Statement														
End of Year	1	2	3	4	5	6	7	8	9	10	11	12	13	14
Revenue			$110,726,832.82	$110,726,832.82	$110,726,832.82	$110,726,832.82	$110,726,832.82	$110,726,832.82	$110,726,832.82	$110,726,832.82	$110,726,832.82	$110,726,832.82	$110,726,832.82	$110,726,832.82
		$11,800,000	$10,113,780.00	$7,223,960.00	$5,160,140.00	$3,686,320.00	$2,632,580.00	$1,580,020.00	$526,280.00	$0.00	$0.00	$0.00	$0.00	$0.00
Expenses														
Materials			$69,867,017	$69,867,017	$69,867,017	$69,867,017	$69,867,017	$69,867,017	$69,867,017	$69,867,017	$69,867,017	$69,867,017	$69,867,017	$69,867,017
Labor			$805,000	$829,150	$854,025	$879,645	$906,035	$933,216	$961,212	$990,048	$1,019,750	$1,050,342	$1,081,853	$1,114,308
Utilities			$1,793,035	$1,793,035	$1,793,035	$1,793,035	$1,793,035	$1,793,035	$1,793,035	$1,793,035	$1,793,035	$1,793,035	$1,793,035	$1,793,035
Catalyst		$753,982				$753,982				$753,982				
Others			$19,998,462	$20,040,241	$20,083,274	$20,127,598	$20,173,252	$20,220,275	$20,268,709	$20,318,596	$20,369,979	$20,422,904	$20,477,417	$20,533,565
Depreciation			0.1429	0.2449	0.1749	0.1249	0.0893	0.0892	0.0893	0.0446				
Building			$1,686,220	$2,889,820	$2,063,820	$1,473,820	$1,053,740	$1,052,560	$1,053,740	$526,280	$0	$0	$0	$0
Machines			$0.00	$0.00	$0.00	$0.00	$0.00	$0.00	$0.00	$0.00				
Tools														
Taxable Income			$16,577,099	$15,307,569	$16,065,662	$16,585,717	$16,933,754	$16,860,730	$16,783,120	$17,231,857	$17,677,052	$17,593,534	$17,507,511	$17,418,907
Income Taxes			$7,459,694	$6,888,406	$7,229,548	$7,463,573	$7,620,189	$7,587,329	$7,552,404	$7,754,335	$7,954,673	$7,917,090	$7,878,380	$7,838,508
Net Income			$9,117,404	$8,419,163	$8,836,114	$9,122,145	$9,313,565	$9,273,402	$9,230,716	$9,477,521	$9,722,378	$9,676,444	$9,629,131	$9,580,399
Cash Flow Statement														
Operating Activities														
Net Income			$9,117,404	$8,419,163	$8,836,114	$9,122,145	$9,313,565	$9,273,402	$9,230,716	$9,477,521	$9,722,378	$9,676,444	$9,629,131	$9,580,399
Depreciation			$1,686,220	$2,889,820	$2,063,820	$1,473,820	$1,053,740	$1,052,560	$1,053,740	$526,280	$0	$0	$0	$0
Investment Activities														
Land														
Buildings	$7,080,000	-$4,720,000												
Machines	$0.00	$0												
Tools														
Gains Tax														
Land														-$531,000
Buildings														$0
Machines														$1,180,000
Tools														
Working Capital		-$11,845,752.83	-$6,037.50	-$6,218.63	-$6,405.18	-$6,597.34	-$6,795.26	-$6,999.12	-$7,209.09	-$7,425.36	-$7,648.12	-$7,877.57	-$8,113.90	$11,923,079.90
Net Cash Flow	-$7,080,000.00	-$16,841,764.83	$10,797,586.87	$11,302,764.52	$10,893,528.90	$10,589,367.21	$10,360,509.67	$10,318,962.49	$10,277,246.82	$9,996,375.74	$9,714,730.25	$9,668,566.17	$9,621,017.17	$22,152,478.91
Cummulative Cash Flow	-$7,080,000.00	-$23,921,764.83	-$13,124,177.96	-$1,821,413.44	$9,072,115.47	$19,661,482.68	$30,021,992.35	$40,340,954.84	$50,618,201.66	$60,614,577.40	$70,329,307.65	$79,997,873.82	$89,618,890.99	$111,771,369.90
Present Value	-$6,321,428.57	-$13,426,151.81	$7,685,509.06	$7,183,111.19	$6,181,280.85	$5,364,902.98	$4,686,568.42	$4,167,655.88	$3,706,078.23	$3,218,565.45	$2,792,752.80	$2,481,680.12	$2,204,888.82	$4,532,836.08
Cumul Discounted CF	-$6,321,428.57	-$19,747,580.38	-$12,062,071.32	-$4,878,960.13	$1,302,320.72	$6,667,223.70	$11,353,792.12	$15,521,448.00	$19,227,526.23	$22,446,091.69	$25,238,844.49	$27,720,524.61	$29,925,413.43	$34,458,249.52

Net Present Value

MARR(12%)	$34,458,249.52

Appendix H: References

[1] Migniot, Jacques. *ETHYLBENZENE : ENVIRONMENTAL, HEALTH & SAFETY GUIDELINES.* CEFIC. 12 December 2012. http://www.ethylbenzene.org/content/1-2.html

[2] Turton, Richard. *Analysis, Synthesis, and Design of Chemical Processes.* Upper Saddle. River, NJ: Prentice Hall, 2012. Print

[3] Wiley, Ron, Joe Bernardi, Joe Louvar, Dennis Hendershot, Dan Crowl, Ralph W. Pike, Amy Theis, and Robert Johnson. *Sache - Student Certificate Program*. Rep. American Institute of Chemical Engineers, Safety and Chemical Engineering Education Program, n.d. Web. 01 Dec. 2014. <http://sache.org/student_certificate_program.asp>.

[4] Perry, Robert H., Don W. Green, James O. Maloney. *Perry's Chemical Engineers' Handbook.* New York: McGraw-Hill, 1984. Print.